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Economics of distillation schemes for ternary mixtures with small light ends concentration

Nickos Doukas
Lehigh University

ECONOMICS OF DISTILLATION SCHEMES FOR TERNARY MIXTURES WITH SMALL LIGHT ENDS CONCENTRATIONS

by

Nickos Doukas

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(date)

W. L. Luyben
Dr. W. L. Luyben
Professor in Charge

Dr. L. A. Wenzel
Chairman, Department
of Chemical Engineering

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Table of Contents

List of Figures

List of Tables

ABSTRACT

Steady state economic evaluations of four different distillation column configurations were made: two conventional columns and a sidestream column with or without a prefractionator. The schemes were examined under different feeds of the same ternary system, i.e. benzene - toluene - o-xylene, where the lightest component was in low concentrations and the other two in equal amounts.

This system was chosen because of its industrial importance and because it exhibits constant relative volatilities (6.7:2.4:1). It was found that a single sidestream column is the most economic one when the concentration of benzene in the feed is lower than 10 percent. The sidestream column with prefractionator scheme is the best one for concentrations of benzene between 10-33 percent.

A single sidestream column remains the most economic one, at low concentrations of the lightest component, even when the relative volatilities are as low as 3:2:1.

CHAPTER ONE: INTRODUCTION

1.1 Energy Consumption in Distillation

Distillation columns are in common use in the chemical and petrochemical industries. These systems consume large amounts of energy for a given separation. With the low cost of energy of the last decade that was not a major problem. With the increasing energy cost nowadays, energy consumption is a major problem. It has become desirable to operate distillation columns in a more efficient way.

Several authors have described different schemes for minimizing energy consumption in multicomponent distillation processes. King (1971) discusses the method where for a given separation of N components at high purities we need N-1 column. Petlyuk et. al. (1965) proposes different schemes for achieving a given separation of a multicomponent system. They examined a ternary system A, B, C with very low relative volatilities, i.e., 1.2:1.1:1.0 respectively, and concluded that the prefractionator case is the most economical if the feed's composition of component B is greater than .3, and the compositions of the other two are equal.

Rathore et. al. (1974) proposed a method for the most economical sequence of N-1 conventional distillation columns, when a multicomponent mixture of N components is to be

separated at high purities. They considered energy integration and assumed that the columns are operating at optimum pressure.

Nishimura et. al. (1971) discussed a method for an economically optimal pattern of separation of multicomponent systems through a sequence of conventional columns. Stupin et. al. (1972) compared a thermally coupled system with the conventional schemes, proposed by King, for a multicomponent separation and showed that it is of lower cost, when the relative volatilities of the components were 9:3:1.

1.2 Scope of this Work

This work is concerned with an economic study of a given ternary system when a specified separation is desirable. We have examined (1) the conventional two-column schemes, (2) the single-column sidestream case, and (3) the prefractionator system, where its products are fed into a sidestream column.

We have tested those schemes for different feeds, where we always kept the most volatile component in low concentrations (lower than 33 percent), and we had equal amounts of the other two components.

From the results some general conclusions can be drawn

for the best configuration for the similar cases. The assumptions made for this study are:

(1) Ideal states, i.e., 100 percent efficiency.

(2) All the columns operate under atmospheric pressure, and there is no pressure drop along the columns.

(3) The vapor leaving a tray, which is in equilibrium with the liquid on the tray, is an ideal gas.

CHAPTER TWO: STEADY STATE DISTILLATION TECHNIQUES

2.1 Introduction

A conventional distillation column is defined as one that has one feed and two product streams, the distillate and the bottoms, while a complex column has either more feeds or streams withdrawn or a combination of these.

Generally a stage in a distillation column can be represented as shown in Figure 1. If we have a conventional column, then LS = 0 and LV = 0 for all trays and F = 0 but for the feed plate. The equations describing this complex ideal stage, and therefore with some simplications describing each one of the stages of a distillation column, are the following:

Equilibrium:

$$Y(N,J) = K(N,J) * X(N,J) \tag{1}$$

$$\sum_J Y(N,J) = 1 \tag{2}$$

or $$\sum_J X(N,J) = 1 \tag{3}$$

Material balance

$$F(N) * Z(N,J) + L(N+1) * X(N+1,J) + V(N-1) * Y(N-L,J) = [V(N)+LV(N)] * Y(N,J) + [L(N)+LS(N)] * X(N,J) \tag{4}$$

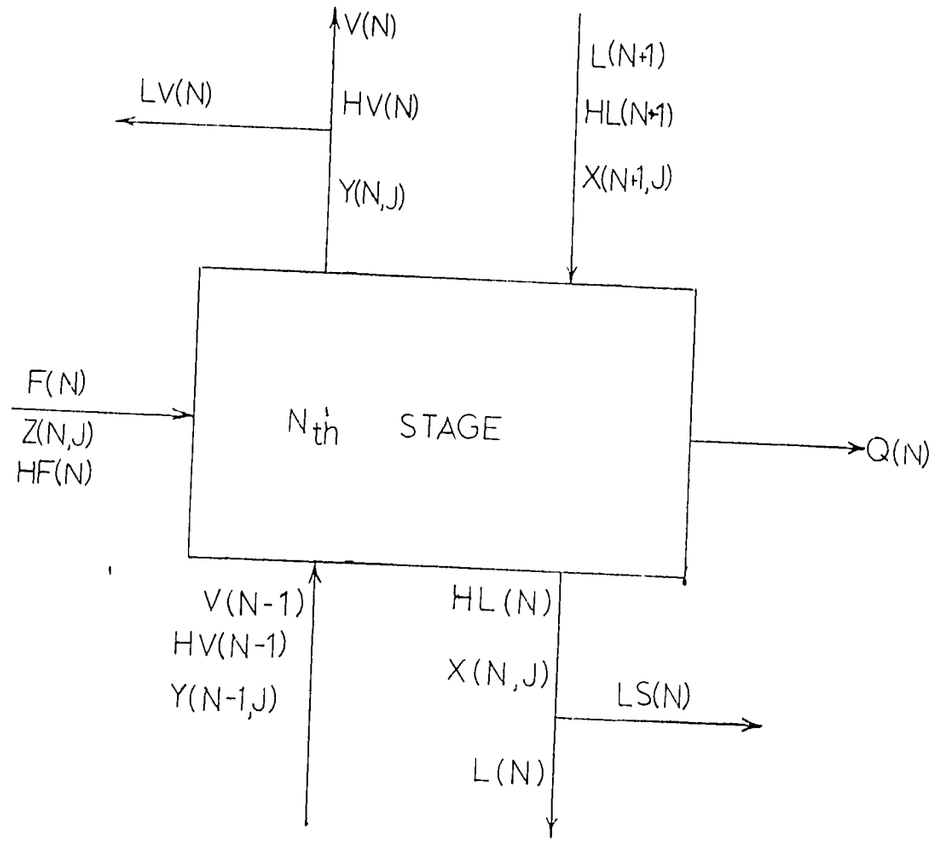

Figure 1 - Ideal equilibrium stage

Enthalpy balance

$$L(N+1) * HL(N+1) + V(N-1) * HV(N-1) + F(N) * HF(J) = [V(N)+LV(N)] * HV(J) + [L(N) + LS(N)] * HL(J) + Q(N) \quad (5)$$

Those four sets of equations are the necessary ones for describing completely an ideal equilibrium stage where we have a vapor stream entering a stage and a liquid stream leaving it.

2.2 Vapor - Liquid Equilibrium

If the liquid compositions of a stage are known, then the vapor compositions are calculated through a bubble point temperature calculation.

We assumed that the vapor leaving a tray is an ideal gas, where the K values for each component are given by:

$$K(J) = A(J) + B(J) * T + C(J) * T^2 + D(J) * T^3$$

The procedure that we follow to evaluate the Y(N,J) when we know X(N,J) is:

(1) Guess a temperature (T).

(2) Evaluate K(J).

(3) Evaluate Y(N,J) through equation (1).

(4) Check if equation (4) is satisfied for the set of Y's we have just calculated.

(5) A. Yes. Then we know the Y's and temperature of the tray.

B. No. Change the guess of T and go back to Step 2.

Vapor - liquid equilibrium is evaluated by subroutine EQUIL, where the new guesses of temperature are performed through Newton-Raphson iterations.

2.3 Numerical Techniques

2.3.1 Wang-Henke Method

This method was first presented in a paper by J. C. Wang and G. E. Henke (1966).

According to this method we write the material balance equations for one component throughout the column, assuming that we only have one feed on tray NF, and a liquid sidestream from tray NS. Our column has NT trays plus a condenser and a reboiler.

Then we have for component #1 for example:

```
(-VB*KB(1)-BOT) * XB(1) + L(1) * X(1,1) = 0          reboiler

VB * KB(1) * XB(1) + (-L(1)-V(1)*K(1,1))
* X(1,1) + L(2) * X(2,1) = 0                          tray 1

V(N-1) * K(N-1,1)*X(N-1,1) + (-L(N)-V(N)*K(N,1))
* X(N,1) + L(N+1) * X(N+1,1) = 0          stripping and
                                          rectifying section
```

but

$$V(NF-1)*K(NF-1,1)*X(NF-1,1) + (-L(NF)-V(NF)*K(NF,1)) * X(NF,1) + L(NF+1) * X(NF+1,1) = -FL * XF(1)$$ feed tray

$$V(NF)*K(NF,1)*X(NF,1) + (-L(NF+1)-V(NF+1)*K(NF+1,1)) * X(NF+1,1) + L(NF+2) * X(NF+2,1) = -FV * YF(1)$$ tray above the feed tray

$$V(NS-2)*K(NS-2,1)*X(NS-2,1) + (-L(NS-1)-V(NS-1) *K(NS-1,1)) * X(NS-1,1) + (L(NS)-LS) * X(NS,1) = 0$$ tray below sidestream tray

$$V(NT-1)*K(NT-1,1)*X(NT-1,1) + (R*K(NT,1)-V(NT) *K(NT,1)=L(NT)) * X(NT,1) = 0$$ tray NT

or in a matrix notation

$$
\begin{bmatrix}
A(1) & B(1) & & & & & & & \\
C(2) & A(2) & B(2) & & & & & & \\
 & C(N) & A(N) & B(N) & & & & & \\
 & & C(NF+1) & A(NF+1) & B(NF+1) & & & & \\
 & & & C(NF+2) & A(NF+2) & B(NF+2) & & & \\
 & & & C(N) & A(N) & B(N) & & & \\
 & & & & C(NS) & A(NS) & B(NS) & & \\
 & & & & & C(N) & A(N) & B(N) & \\
 & & & & & & C(NT+1) & A(NT+1)
\end{bmatrix}
\begin{bmatrix}
XB(1) \\ X(1,1) \\ X(N-1,1) \\ X(NF,1) \\ X(NF+1,1) \\ X(N-1,1) \\ X(NS-1,1) \\ X(N-1,1) \\ X(NT,1)
\end{bmatrix}
=
\begin{bmatrix}
0 \\ 0 \\ 0 \\ -FL*XF(1) \\ -FV*YF(1) \\ 0 \\ 0 \\ 0 \\ 0
\end{bmatrix}
$$

where C is the first coefficient of the equation, A is the second one, and B the third one. Note that the reboiler equation does not have a C coefficient, while the top tray equation does not have a B term. Thomas' algorithm is used to solve this matrix (Lapidus, 1962). Two new variables W and G are calculated as follows:

$$W(1) = A(1)\ ,\ g(1) = D(1)/W9_1)$$

$$W(N) = A(N) - C(N) * B(N-1)/W(N-1) \qquad 2 \leq N \leq NT+1$$

$$G(N) = (D(N) - C(N) * G(N-1)/W(N)$$

Then we have:

$$X(NT,1) = G(NT+1)$$

$$X(N-1,1) = G(N) - X(N+1) * B(N)/W(N) \qquad 2 \leq N \leq NT$$

$$XB(1) = G(1) - X(2) * B(1)/W(1)$$

Then we go through the same calculations again for each of the other components, changing the coefficients in the matrix for each component.

The steps to be followed for computing the steady state vapor and liquid profiles as well as the tray compositions are the following:

(1) Set D, R, LS with NT, NF, NS and feed condition given.

(2) Guess initial temperatures, vapor and liquid rates for all the trays.

(3) For each component solve for the X's on all trays by forming the tridiagonal matrix.

(4) Adjust all the X's on each tray either by normalization, or by the theta-method,to be described later,so that they sum up to one.

(5) Calculate new Y's and temperatures by bubble point calculations. Then calculate enthalpies.

(6) Calculate vapor and liquid rates from tray to tray enthalpy balances, starting at the top of column where R and D are known.

(7) Find the sum of temperatures (TSUM) on all trays. (If it is the first iteration, skip the other steps and go back to step 4).

(8) Compare the TSUM with the one from the previous iteration. If their difference is smaller than a specified tolerance (.001°F), the system has converged and the values that have been calculated are the ones we are seeking. If the difference of the two values is greater that the tolerance then go back to step 3 and repeat.

2.3.2 Theta Method

This method was presented by C. D. Holland and M. S. Kuk (1975), and for a fixed reflux ratio we will describe it for two different distillation columns:

(1) For a conventional column

Since and we are working with a fixed distillate rate the overall material balance should satisfy

the equations:

$$F * XF(J) = DIST * XD(J) + BOT * XB(J) \tag{6}$$

$$\sum_{1}^{J} XD(J) = 1 \tag{7}$$

Instead of using normalization and successive substitution, using the X's that we calculate through the Wang-Henke method, we define an improved set of X's by defining:

$$\left(\frac{XB(J)}{XD(J)}\right)_{NEW} = \theta * \left(\frac{XB(J)}{XD(J)}\right)_{OLD} \tag{8}$$

where the old values come from the tridiagonal matrix. From equations (6) and (8) we get that

$$NEW\ XD(J) = \frac{F * XF(J)}{\left(\left(1 + \theta * \left(\frac{BOT}{DIST}\right) * \left(\frac{XB(J)}{XD(J)}\right)_{OLD}\right) * DIST\right)} \tag{9}$$

We choose θ so that the new values of XD(J) satisfy equation (7).

We solve this problem by using Newton-Raphson method for the function:

$$FNR = \sum_{J=1}^{NJ} NEW\ XD(J) - 1$$

The derivative is:

$$FNRSL = \sum_{J=1}^{NJ} \frac{DFNR}{D\theta} = -\sum_{J=1}^{NJ} \frac{NEW\ XD(J) * \left(\frac{BOT}{DIST}\right) * \left(\frac{XB(J)}{XD(J)}\right)OLD}{\left(1 + \theta * \left(\frac{BOT}{DIST}\right) * \left(\frac{XB(J)}{XD(J)}\right)_{OLD}\right)}$$

The problem is solved by trial and error where the new guess of θ is given by

$$\theta_{NEW} = \theta_{OLD} - \frac{FNR}{FNRSL}$$

Using the Newton-Raphson method for convergence, one has to start with $\theta = 0$.

After getting the correct θ and all the XD's from equation (4), we calculate the new XB's from equation (3).

The calculation of new X's on all trays is based on their old values that come from the tridiagonal matrix, and the new value of XD, and is given by

$$X(N,J) = \frac{\left(\frac{X(N,1)}{XD(J)}\right)_{OLD} * NEW\ XD(J)}{\sum_{J=1}^{NJ} \left(\frac{X(N,J)}{XD(J)}\right)_{OLD} * NEW\ XD(J)}$$

Table 1 gives a comparison of the number of iterations needed for the same system to converge for different reflux ratios.

Figure 2 shows how the final value of theta changes from iteration to iteration, while Figure 3 shows how rapidly XD converges to the correct value

(2) For a sidestream column

For the sidestream column equation (7) remains the same as before but equation (6) becomes

$$F* XF(J) = DIST * XD(J) + BOT * XB(J) + LS * XS(J) \quad (10)$$

Table 1

Comparison of number of iterations needed for a system to converge by using successive substitution or θ-method.

First System

R/D	Successive Substitution	θ- Method
14.584	102	37
14.084	76	32
14.155	22	14
14.155	19	10
14.155	15	8

Second System

1.94	46	22
1.84	34	19
1.89	36	19
1.87	33	17
1.85	30	17
1.86	29	17
1.865	28	16
1.8625	27	15
1.86375	20	12
1.863125	17	11
1.863	12	9
1.863	9	7
1.863	2	7

First System: NT=27, NF=10, XF1=.10, XF2=.45, XF3=.45
BOT=91.95, DIST=8.05, F=100

Second System: NT=19, NF=10, XF1=.03, XF2=.49, XF3=.49
BOT=44.892, DIST=47.059, F=91.95

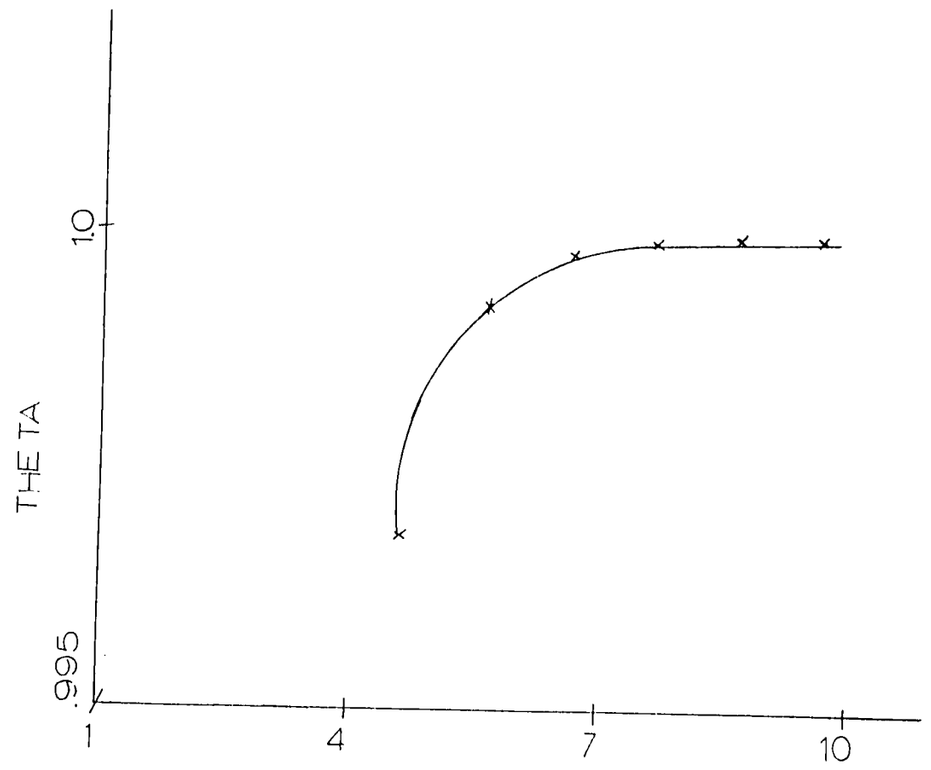

Figure 2 - θ vs. number of iterations

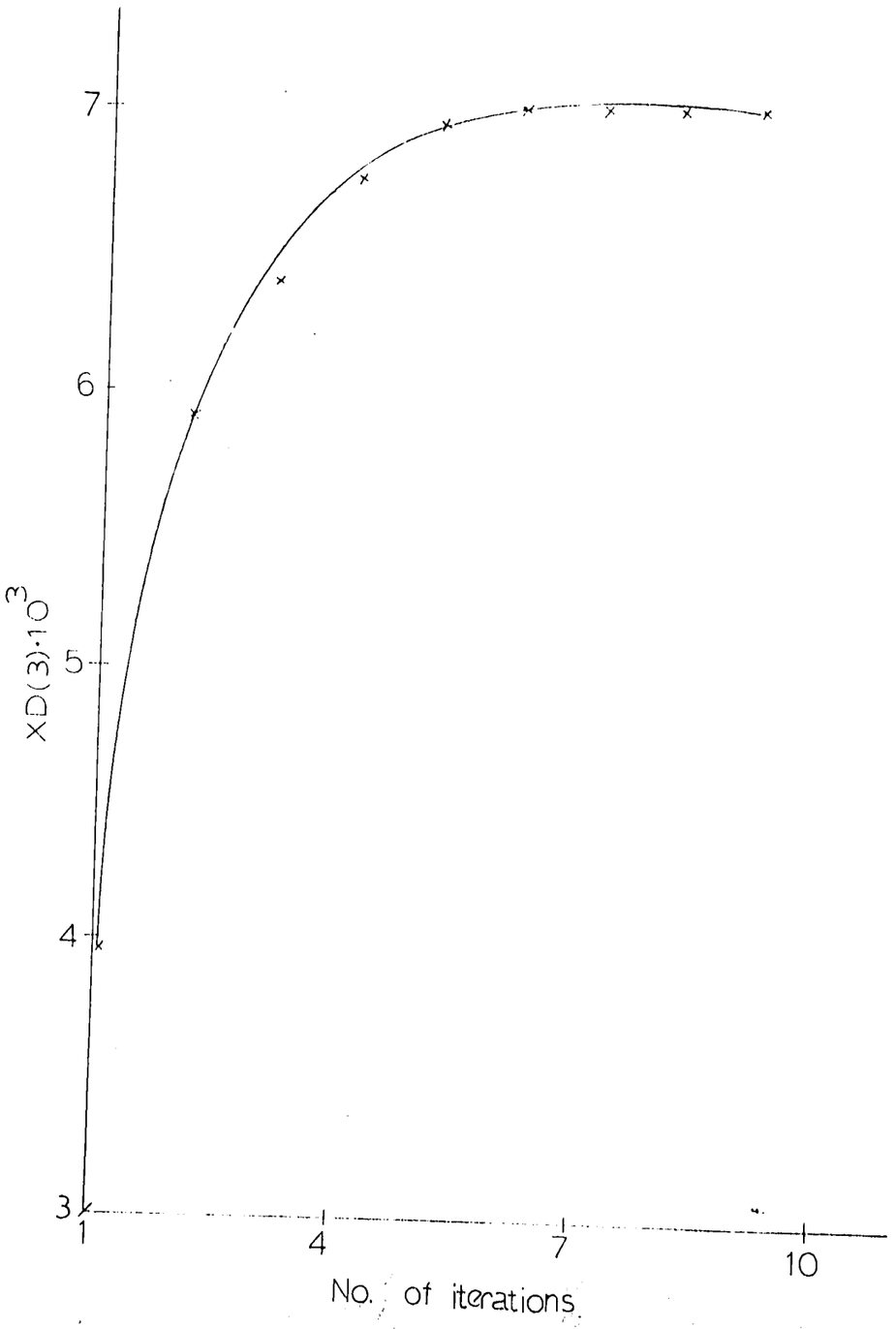

Figure 3 - XD(3) vs. number of iterations

If the flowrates are fixed, then using the values for X's that come from the tridiagonal matrix we define the improved values of X's as follows:

$$\left(\frac{XB(J)}{XD(J)}\right)_{NEW} = \theta 1 * \left(\frac{XB(J)}{XD(J)}\right)_{OLD} \tag{11}$$

$$\left(\frac{XS(J)}{XD(J)}\right)_{NEW} = \theta 2 * \left(\frac{XS(J)}{XD(J)}\right)_{OLD} \tag{12}$$

From equations (10), (11) and (12) we get

$$\text{NEW XD(J)} = F * XF(J) /$$

$$\left((1+\theta 1*\left(\frac{BOT}{DIST}\right)*\left(\frac{XB(J)}{XD(J)}\right)_{OLD}+\theta 2*\left(\frac{LS}{DIST}\right)+\left(\frac{XS(J)}{XD(J)}\right)_{OLD}\right) * DIST)$$

From equation (12) we can get the new value for XS(J).

Now we have to find two thetas, instead of one that we had before. We will calculate them using Newton-Raphson method but this time the initial guesses of both thetas should be equal to one for the method to converge.

We define our Newton-Raphson functions as:

$$FNR1 = \sum_{J=1}^{NJ} \text{NEW XD(j)} - 1$$

$$FNR2 = \sum_{J=1}^{NJ} \text{NEW XS(J)} - 1$$

The partial derivatives of those functions with respect to $\theta 1$ and $\theta 2$ can be calculated explicitly and after this we find the Jacobian of them:

$$Q = \begin{vmatrix} \frac{\partial FNR1}{\partial \theta 1} & \frac{\partial FNR1}{\partial \theta 2} \\ \frac{\partial FNR2}{\partial \theta 1} & \frac{\partial FNR2}{\partial \theta 2} \end{vmatrix}$$

Knowing the values of the Newton-Raphson functions for values of the two thetas, as well as Q, we calculate the changes of the thetas as:

$$D\theta 1 \quad (FNR2 * \frac{\partial FNR1}{\partial \theta 2} - FNR1 * \frac{\partial FNR2}{\partial \theta 2})/Q$$

$$D\theta 2 = (FNR1 * \frac{\partial FNR2}{\partial \theta 1} - FNR2 * \frac{\partial FNR1}{\partial \theta 1})/Q$$

keeping always in mind that the new thetas should be always positive. If they turn out to be negative we simply halve their previous value. After getting the correct values of thetas, we know the new values of XD, XS and XB and we calculate the rest X's from the equation:

$$X(N,J) = \frac{(\frac{X(N,J)}{XD(J)})_{OLD} * NEWXD(J)}{\sum_{J=1}^{NJ} (\frac{X(N,J)}{XD(J)})_{OLD} * NEWXD(J)}$$

Table 2 shows how the final values of thetas change from iteration to iteration, while Figure 4 shows how XD

converges to the correct value. The use of θ-method requires less computer time for a system to converge. For example the program of a specific distillation scheme, with and without the use of θ-method, requires 17.7 and 21.9 system seconds to converge to the desired XD value. Meanwhile the system has converted for 45 different reflux ratios. Therefore, for a fixed reflux ratio the computer time required, without the compilation time, is approximately .4 seconds

Table 2

Changes of θ in a two-θ method

Iteration	θ1	θ2
1	.485271	2.084351
2	1.234856	1.241550
3	1.496103	1.041391
4	.868432	1.006176
5	.916297	1.0015
6	1.079786	1.00056
7	1.032393	.999864
8	.999912	.999874
9	1.018276	.999977
10	1.023212	.999939
11	1.017946	.999918
12	1.017662	.999929
13	1.019167	.999932
14	1.018962	.999928
15	1.018602	.999928
16	1.018730	.999929
17	1.018804	.999929

System: Sidestream column with two feeds.

NT=45 NF=39 XF(1)=.1658 XF(2)=.8272 XF(3)=.0070

NS=38 NF1=25 XF1(1)=.0024 XF1(2)=.3301 XF1(3)=.6675

RR=41.0163 BOT=284.21 DIST=15.79 LS=300.00

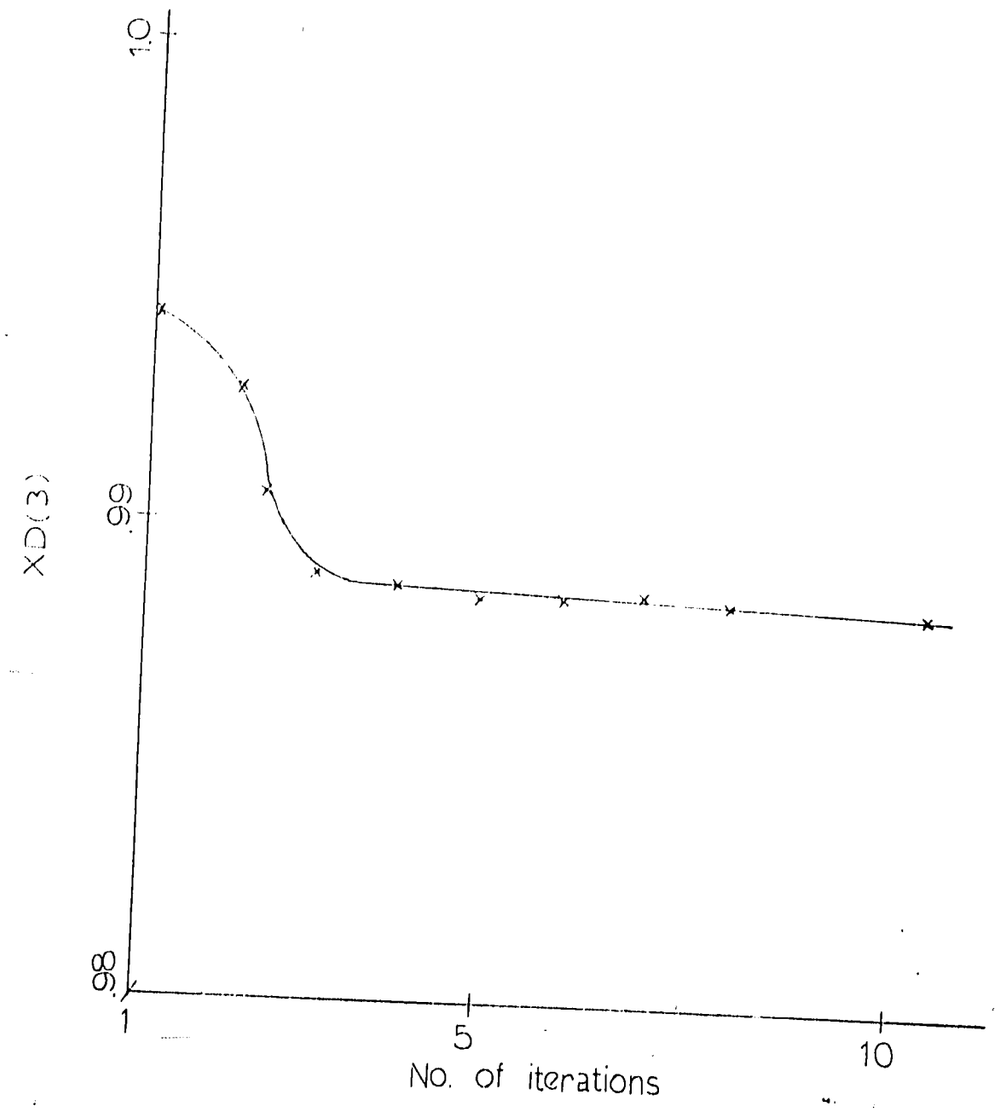

Figure 4 - XD(3) vs. number of iterations for SSC

CHAPTER THREE: ECONOMIC BASES

3.1 Introduction

There have been several known schemes for a multi-component distillation which have not been used significantly earlier due to low energy costs. With the shortage of fuels and the increasing cost of energy these schemes have become more profitable.

In this work we want to achieve a certain separation of a given ternary system at minimum cost. The examined system consists of low amounts of benzene, and higher but equal amounts of toluene and o-xylene. Seven different feeds have been examined for this special case where we have components with fairly large relative volatilities. A few cases were also tested for a system with lower relative volatilities.

The desired separation is to produce three product streams:

(1) 95% benzene with 5% toluene

(2) 95% o-xylene with 5% toluene, and

(3) 90% toluene with 5% benzene and 5% o-xylene

The four different schemes tested are:

A. Two conventional columns

(1) Two columns where the top product of the first is the feed of the second (hereafter called "Heavy

Out First" configuration - H.O.F.). From the first column we take o-xylene as the bottoms products, while benzene is the overhead product of the second column, and toluene the bottoms product of the same column. This is shown in Figure 5.

(2). Two columns where the bottom product of the first is the feed of the second (hereafter called "Light Out First" configuration - L.O.F.). From the first column we take benzene as the overhead product, while toluene is the overhead product from the second column, and o-xylene its bottom product. This is shown in Figure 6.

B Sidestream cases

(1) A single sidestream column with a liquid draw-off (hereafter called the "S.S.C." configuration). In this case we have three product streams from the same column. We take benzene as the overhead product, toluene as the sidestream product and o-xylene as the bottom product. A liquid sidestream is removed at a location above the feed tray because there we have low concentrations of o-xylene (heavy key), and of benzene (light key; mainly in vapor stream). This is shown in Figure 7.

(2) A prefractionator/sidestream column configuration (hereafter called the "PSC" configuration). The first column in this case makes a split between

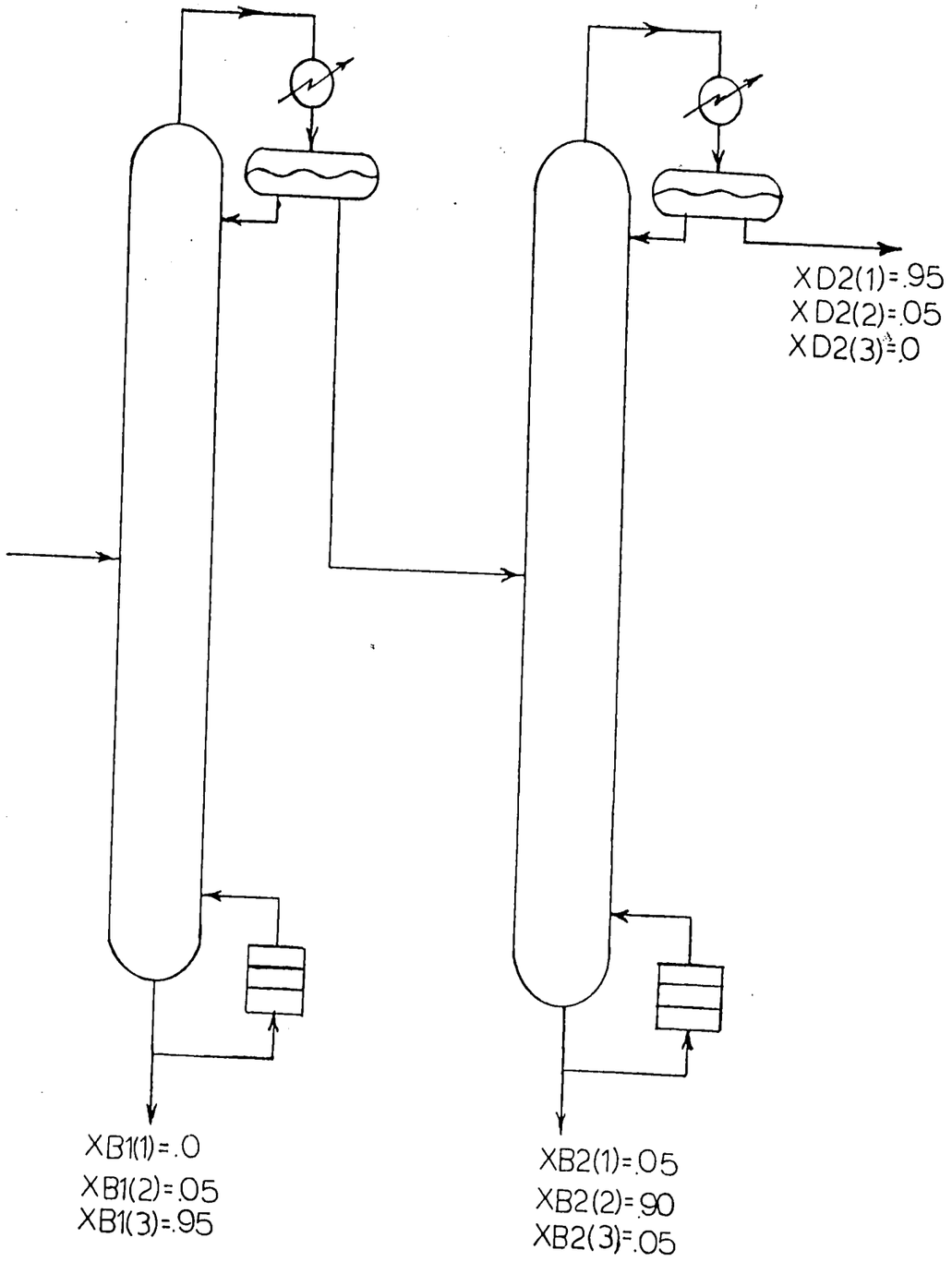

Figure 5 - H.O.F. configuration

Component	No
Benzene	1
Toluene	2
O-xylene	3

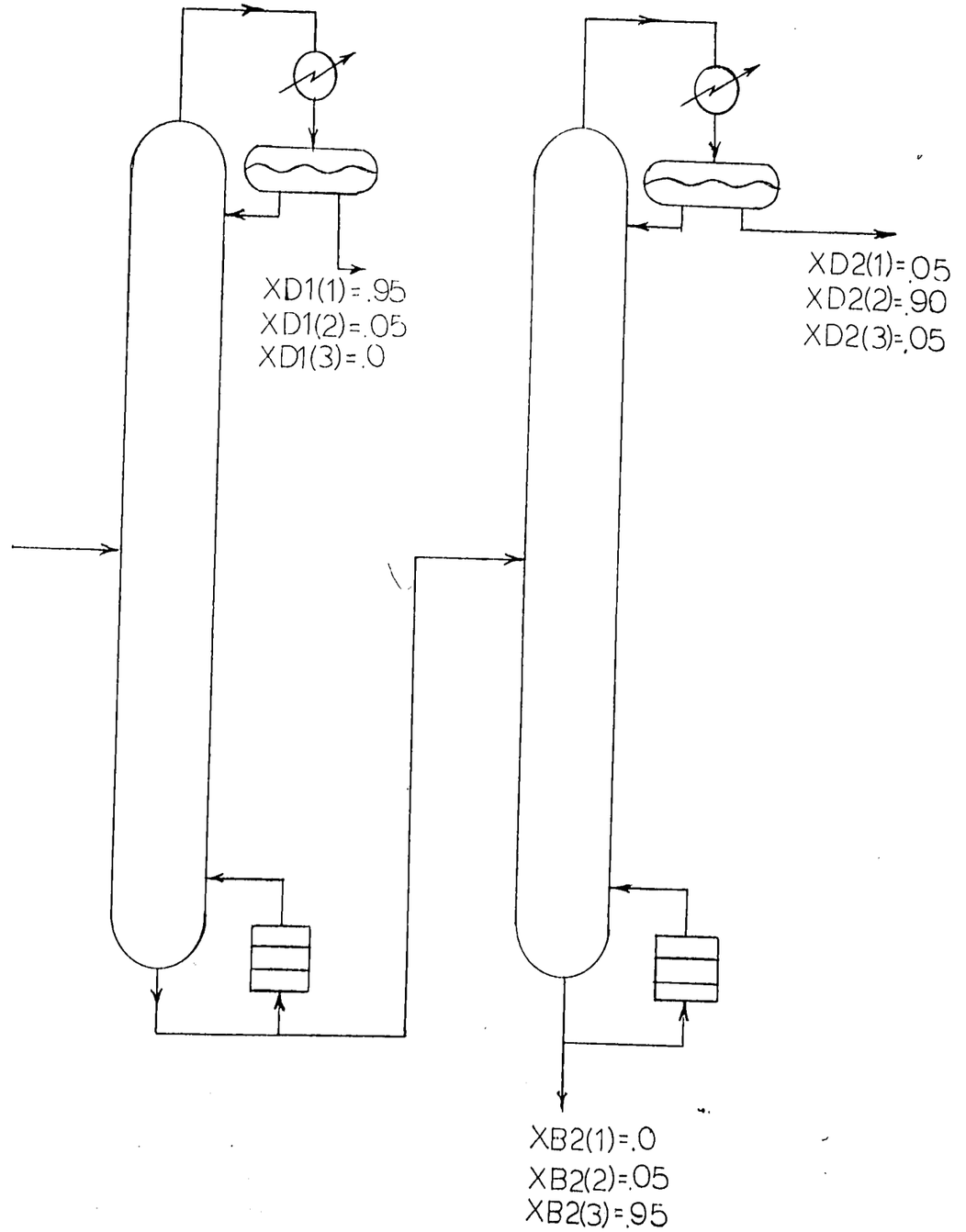

Figure 6 - L.O.F. configuration

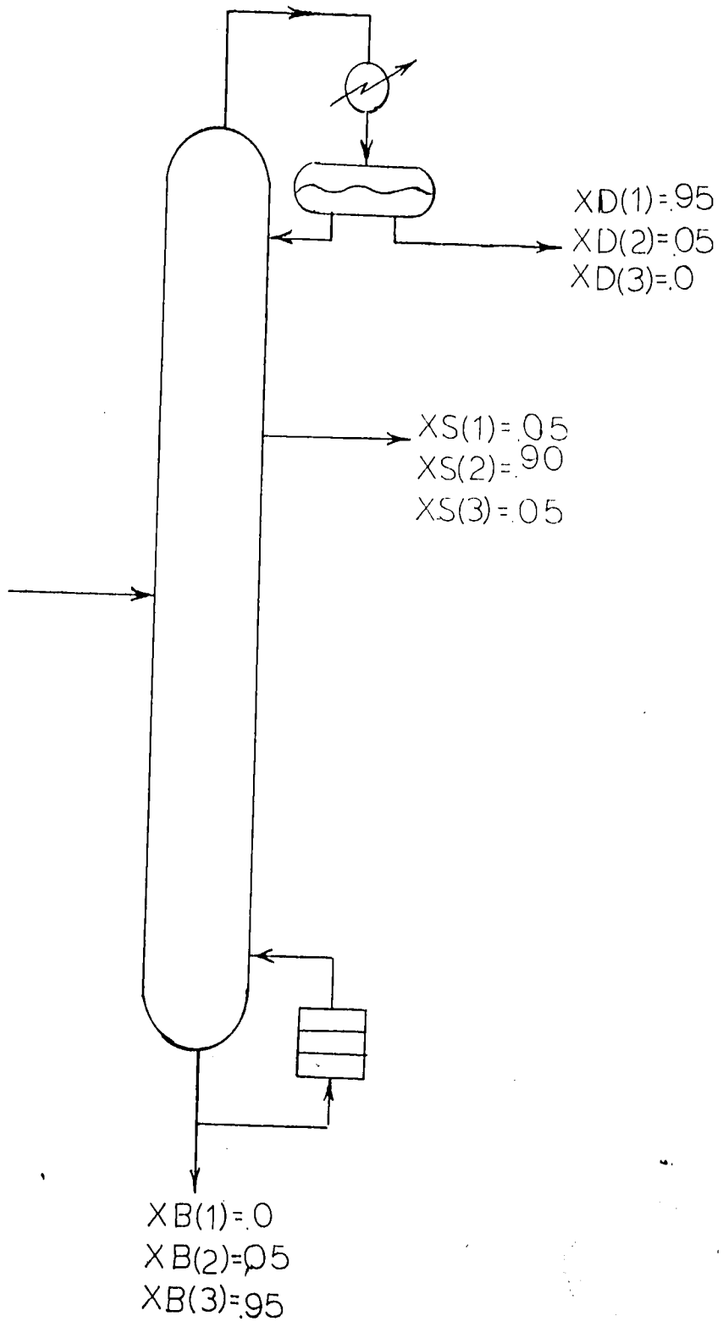

Figure 7 - SSC configuration

the heaviest and the lightest components. The overhead product's composition consists of .5 percent of heavy component and the rest is benzene (almost all the benzene goes out the top) and toluene. The bottoms product's composition consists of .5 percent of benzene. The rest is toluene and o-xylene, (almost all the o-xylene goes out the bottom). The products of this column are fed into the sidestream column at locations above and below the sidestream draw off location. The products of the sidestream column are the same as in the SSC case. This scheme is shown in Figure 8.

3.2 Economic Data

The accuracy of the results obtained in any economic evaluation problem, depends on the cost estimation and the assumptions made. The cost for each one of the tested schemes includes:

(1) The capital cost, which is a function of column's diameter and height, reboiler's and condenser's area, and instrumentation.

(2) The operating cost which is a function of utilities.

A. Capital Cost

The cost of columns and the cost of reboilers and condensers has been calculated from graphs given by

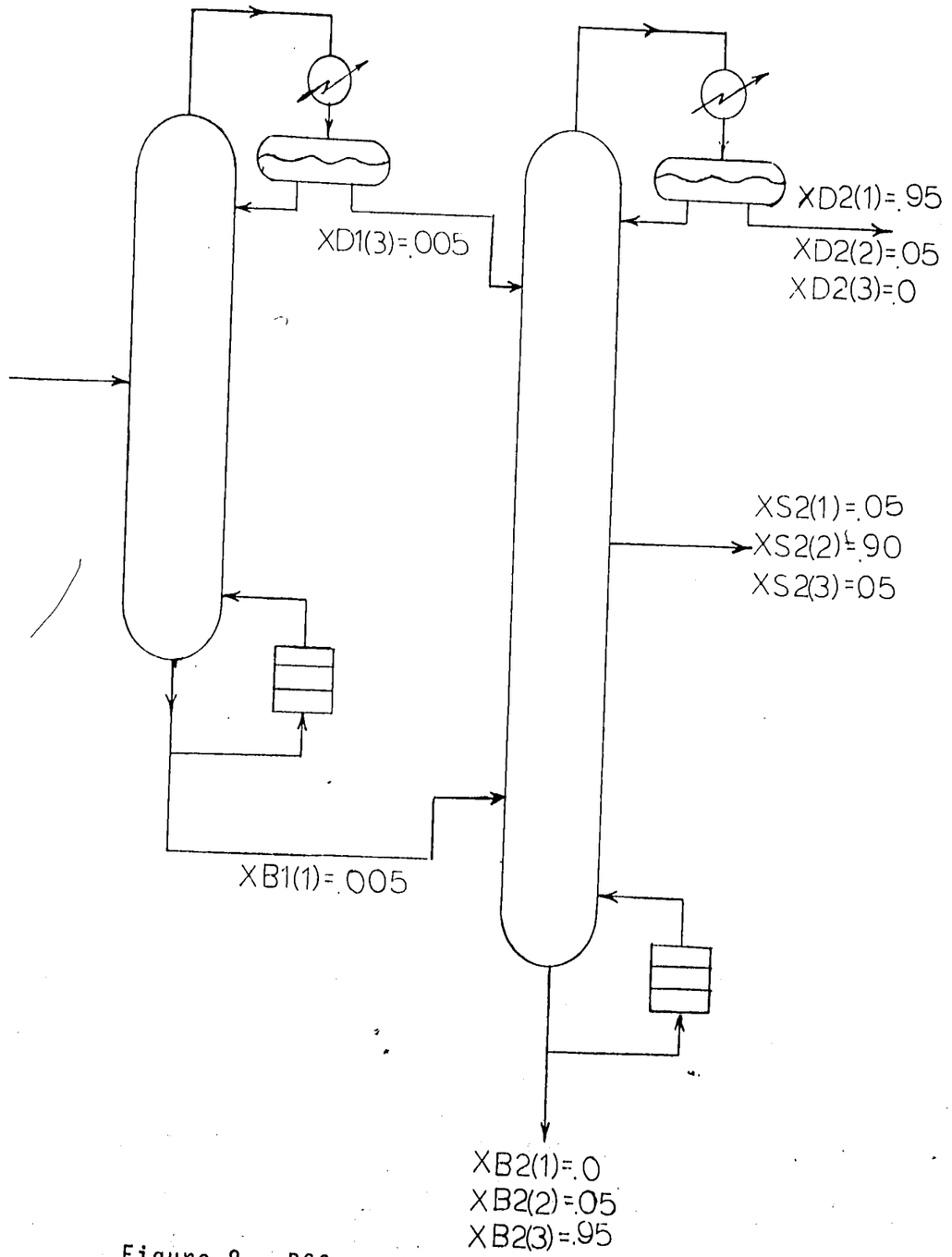

Figure 8 - PSC configuration

Dryden and Furlow (1966). Those graphs are based on estimations made with a Marshall and Stevens Equipment Index (M&S) equal to 270, and they were scaled by a factor 1.637 (present M&S = 442 obtained from Chemical Engineering economic indicators).

Plots of column, reboiler, and condenser cost are given in Figures 9 and 10 respectively.

The sum of costs for piping, insulation and instrumentation is estimated to be 60 percent of the cost for the installed equipment.

Annual fixed charges are 15 percent of the total cost.

B. Operating Cost

The main difficulty was in estimating the cost of utilities, not only because the cost of steam, for example, changes with its pressure, but because it also depends on whether there is steam of the desired pressure available within the plant, or one has to buy the steam from another plant.

The data that we have used in estimating the utilities cost is:

Cooling water at 90°F	$.06/10,000 lb.
200 psig pressure steam	$2.0/1,000 lb.
300 psig pressure steam	$2.2/1,000 lb.

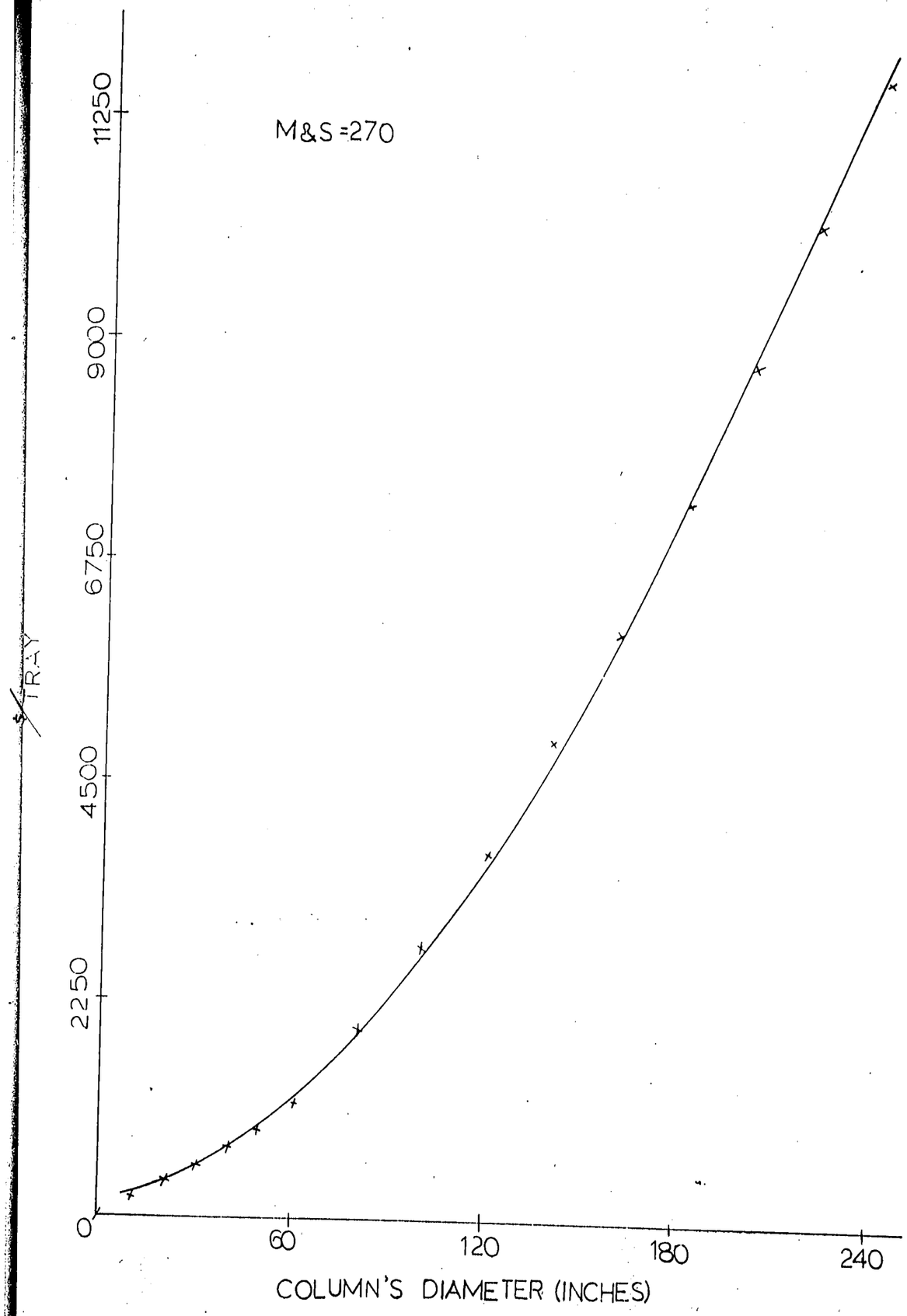

Figure 9 - Cost of column (per tray) in dollars.

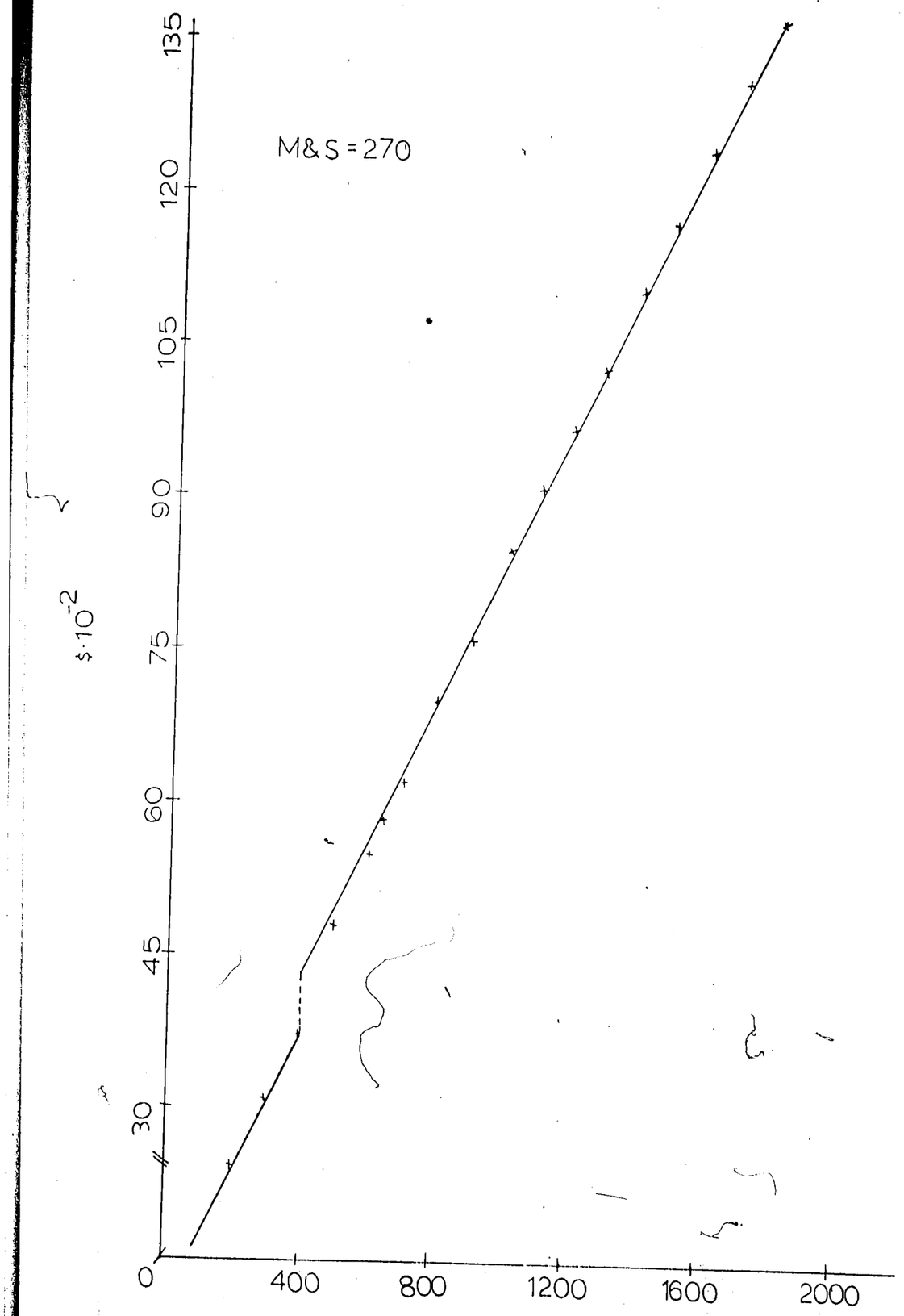

Figure 10 - Cost of heat exchangers in dollars

(Reboiler: multiply times 1.4
Condenser: multiply times 1.21)

3.3 Optimum Reflux Ratio

For a conventional column, we used the Fenske-Underwood equations to calculate the minimum number of trays required, and the minimum reflux ratio for a given separation. Then setting $RR = K * RR_{min}$, where K a constant greater than one and lower than 2, and using the Gilliland correlation we found pairs of actual number of plates required for a given separation and its corresponding reflux ratio.

The cases examined were those with initial feeds consisting of 10 percent benzene, 45 percent toluene and 45 percent o-xylene.

For conventional columns the optimum reflux ratio was found to be about 1.075 times the minimum for all cases. Figure 11 shows the change of annual cost vs. the reflux ratio of the second column of the L.O.F. configuration. (The feed's composition of this column is: 25.6 percent benzene, 48.5 percent toluene, 48.9 percent o-xylene.) Since all these results showed an optimum ratio of close to 1.1, we decided to use $RR_{opt} = 1.1 * RR_{min}$ for all the conventional columns we used.

For sidestream columns we had to find RR_{opt} strictly empirically by evaluating columns with different numbers of trays, different sidestream and feed locations, and

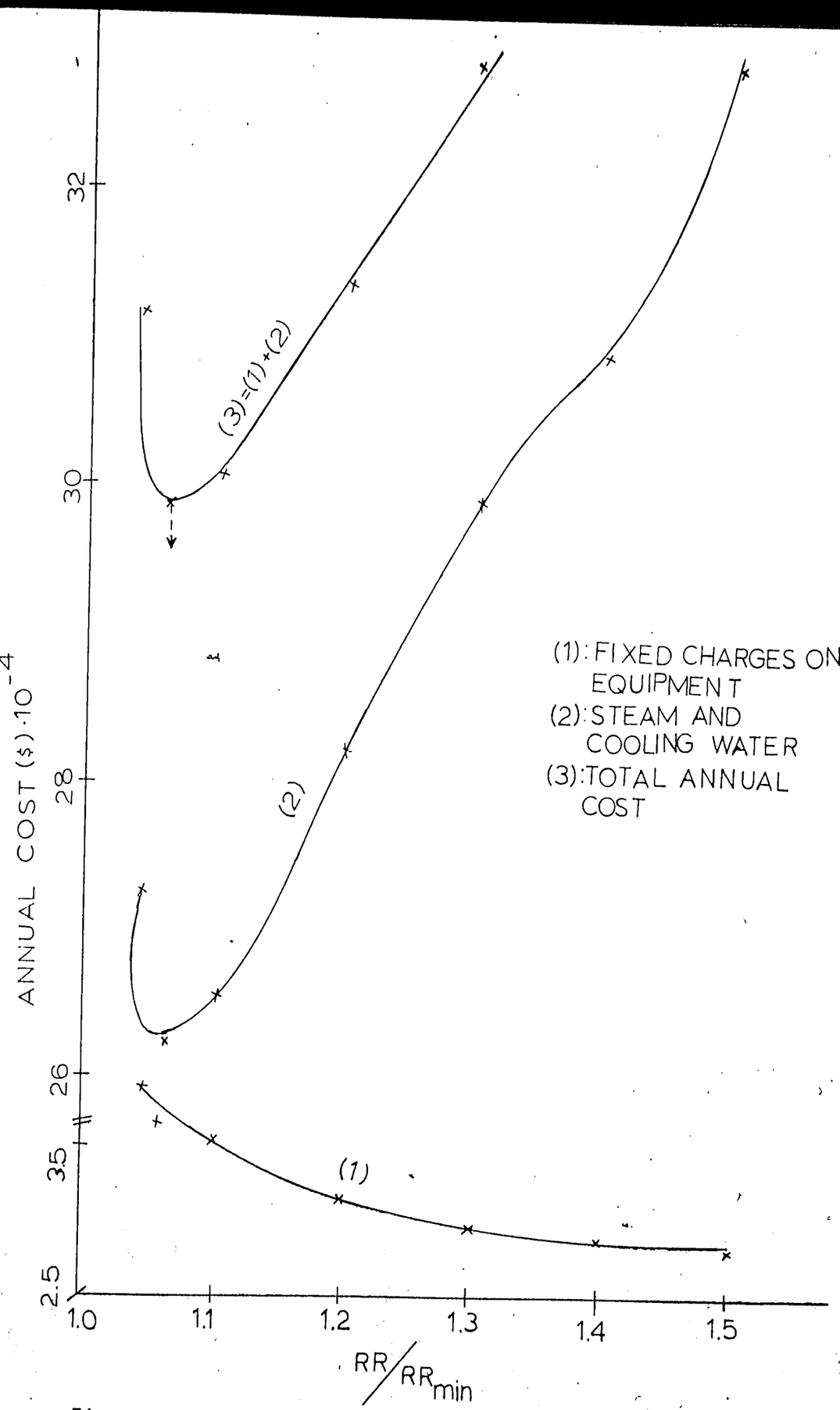

Figure 11 - Cost of the second column of + LOF configuration when XF1=.256, XF2=.485, XF3=.489

different reflux ratios. Economic evaluations had to be made for each single case.

3.4 Description of specific schemes tested

Four different mathematical models were developed and used on the Lehigh University CDC 6400 digital computer, to make rigorous plate to plate calculations for the different schemes examined in this work. The programs take into account the effects of non-equal molar overflow and changes of relative volatilities with composition.

The main assumptions made were that all the columns operate under atmospheric pressure, that there is no pressure drop along the columns, that the plates' efficiency is 100 percent, that all the feeds are saturated liquids, and that we have total condensers and partial reboilers. To evaluate the diameter of the columns we assume a vapor velocity of 2.5 fps at the top of the tower.

We also assume that the overall heat transfer coefficient is 80 Btu/(hr)(sqft)(°F) in the reboiler and 100 Btu/(hr)(sqft)(°F) in the condenser. Finally, we allow a 50°F change in the cooling-water temperature, and we assume that the unit operates 8500 hrs per year.

CHAPTER FOUR: RESULTS AND DISCUSSION

Detailed results for all the examined schemes and feeds are given in Tables 3-6.

Also in Figure 12 the total annual cost for each one of the four schemes tested is plotted as a function of the concentration of benzene in the feed.

The results show that for the given separation of the benzene-toluene-o-xylene system, which has fairly large relative volatilities:

(1) Very low concentrations of the lightest component favor the single sidestream column.

(2) When the concentration of the lightest component is greater than 10 percent, then the PSC configuration is the most economic.

This configuration seems to be the best one even for high concentrations of benzene (lightest component). Even when the benzene concentration in the feed is 33 percent the PSC configuration remains the best one.

The SSC configuration for feeds containing more than 10 percent of benzene is much more expensive. Its cost increases rapidly, due to a drastic increase of the heat input. To maintain the specified sidestream composition, we need higher vapor rates as the amount of benzene in the feed increases. The pinch concentration of benzene in the rectifying section above the feed plate must be kept low or too

Table 3

Results for the H.O.F. configuration

Feed's concentration of benzene		.05		.10		.12	
# of column		1	2	1	2	1	2
Q_D*10^{-6}	Btu/hr	13.0	2.2	12.0	3.7	13.0	4.2
A_D	Sqft	666	148	605	250	671.4	289
Q_B*10^{-6}	Btu/hr	13.0	2.2	12.0	3.7	13.0	4.3
A_R	Sqft	2,353	272	2,079	518	2,275	600
NT		21	20	21	20	24	19
NF		16	11	10	7	19	12
RR		2.1	10.	1.6	5.1	1.8	4.55
Diameter	Inches	106	43.3	99	56.2	103.6	60.5
T_B	°F	346	292	346	292	346	292
T_D	°F	288	237	282	237	279	237
Fixed charges on equipment	$	37,623	9,105	35,456	12,920	40,473	13,394
Steam and cooling water	$	324,209	46,419	286,308	78,804	313,387	91,247
Annual cost of system	$	417,356		413,788		458,501	

Table 3 Continued

.13		.14		.20		.33	
1	2	1	2	1	2	1	2
13.0	4.4	11.0	4.5	11.0	5.45	11.4	6.6
668.4	299.3	592.0	305	615.5	371	671.3	450.4
13.0	4.5	11.4	4.55	11.5	5.55	11.8	6.7
2,265	622	1,991	633.5	2,115.5	772.5	2,068.7	937.7
24	19	24	19	21	17	26	21
19	12	12	7	10	7	21	15
1.7	4.2	1.4	3.8	1.3	2.9	1.14	1.65
103.3	61.6	96.7	62.1	97.2	68.8	98.3	75.5
346	292	346	292	346	292	346	292
278	237	277	237	271	237	260.2	237
36,444	13,093	36,797	13,989	35,809	15,055	38,794	20,931
311,970	94,620	274,161	110,327	276,588	117,505	284,808	142,607
456,127		435,274		444,957		487,136	

Table 4

Results for the L.O.F. configuration

Feed's concentration of benzene		.05		.10		.12	
# of column		1	2	1	2	1	2
Q_D* 10^{-6}	Btu/hr	2.9	11.4	5.0	11.0	5.3	10.0
A_D	Sqft	198	556	338	535	363	516
Q_B* 10^{-6}	Btu/hr	2.9	12.0	5.1	11.0	5.5	11.0
A_R	Sqft	544	2,039	939	1,925	1,015	1,857
NT		20	22	19	22	20	23
NF		6	11	7	11	8	12
RR		13.8	1.8	7.2	1.8	6.0	1.8
Diameter	inches	50.4	99	66	96.1	68.3	94.5
T_B	°F	314	346	314	346	314	346
T_D	°F	237	292	237	292	237	292
Fixed charges on equipment	$	11,144	34,815	17,211	35,475	19,280	33,073
Steam and cooling water	$	62,668	280,811	107,906	265,101	116,502	255,871
Annual cost of system	$	389,508		425,693		424,726	

Table 4 Continued

.13		.14		.20		.33	
1	2	1	2	1	2	1	2
5.5	10.0	5.7	10.0	8.6	9.75	7.4	7.9
377	510	389	503	583.6	482.7	504	392.5
5.7	10.5	5.9	10.0	8.85	9.9	7.8	8.1
1,054	1,759	1,091	1,812	1,634	1,737.6	1,444	1,433
20	23	20	23	17	20	21	21
8	12	8	12	4	10	11	10
5.5	1.8	5.2	1.8	5.1	1.9	2.0	1.9
69.5	93.9	70.7	93.3	86.8	91.7	80.4	82.4
314	346	314	346	314	346	314	346
237	292	237	292	237	292	237	292
18,999	32,928	19,572	32,479	24,168	28,422	24,532	24,373
121,037	252,743	125,227	249,641	187,161	239,356	164,271	194,634
425,707		426,919		479,107		407,810	

Table 5

Results for the S.S.C. configuration

Feed's concentration of benzene	.05	.10	.12	.13	.14	.20	.33
Q_D*10^{-6} Btu/hr	11.0	12.0	14.0	17.0	16.5	30.5	51.0
A_D Sqft	758	810	979	1,134	1,122	2,086	3,460
Q_B*10^{-6} Btu/hr	11.0	12.0	15.0	17.0	17.0	31.0	51.0
A_R	1,995	2,139	2,583	2,983	2,961	5,425	8,992
NT	46	40	42	37	43	30	46
NF	24	20	22	22	20	20	24
NS	39	27	27	26	24	22	25
RR	55.5	28.6	17.8	18.7	16.8	20.7	19.25
Diameter inches	99.5	103	113.1	121.8	121.2	163.2	212.7
T_B °F	346	346	346	346	346	346	346
T_D °F	237	237	237	237	237	236	237
Fixed charges on equipment $	62,622	56,892	68,663	68,867	80,465	103,954	186,073
Steam and cooling water $	274,753	294,570	355,739	410,905	407,827	747,317	1,239,132
Annual cost of system $	337,375	351,462	424,402	479,772	488,292	851,271	1,425,205

Table 6

Results for the P.S.C. configuration

Feed's concentration of benzene		.05		.10		.12	
# of column		1	2	1	2	1	2
Q_D*10^{-6}	Btu/hr	7.25	7.05	5.4	7.88	6.36	7.5
A_D	Sqft	378.7	479.5	300.5	534	360.1	310.5
Q_B*10^{-6}	Btu/hr	7.38	7.175	5.5	8.04	6.56	7.66
A_R	Sqft	1,668	1,256	1,171	1,407	1,416.3	1,341.7
NT		18	45	25	35	19	33
NF		5	39/25	9	30/10	7	30/10
NS		-	38	-	28	-	25
RR		2.09	34.76	1.5	12.04	1.62	8.8
Diameter	inches	78.35	79.2	67	83.6	73.1	81.7
T_B	°F	326.5	346	322.8	346	323.9	346
T_D	°F	281.4	237	268.2	237.6	366.7	237
Fixed charges on equipment	$	22,025	42,537	21,035	37,143	20,347	37,447
Steam and cooling water	$	156,169	173,054	116,933	193,932	138,865	184,777
Annual cost of system	$	393,785		369,043		381,436	

Table 6 Continued

.13		.14		.20		.33	
1	2	1	2	1	2	1	2
5.6	7.85	6.16	7.48	6.33	7.04	6.55	5.9
326.6	533.4	355.4	509	379.8	478.8	415.7	404.8
5.9	8.02	6.4	7.65	6.6	7.20	6.9	6.1
1,227	1,404.5	1,364.3	1,339	1,405.65	1,261.3	1,467.4	1,066.7
20	34	20	33	20	34	21	38
8	32/10	8	30/15	9	32/10	11	36/17
-	26	-	25	-	25	-	27
1.5	8.3	1.48	7.07	1.25	3.98	.84	1.38
69	83.5	71.9	81.6	73.0	79.11	74.7	72.7
322.1	346	323.4	346	323.1	346	322.9	346
263.4	237	263.3	237	256.5	237	247.7	237
19,202	36,325	20,524	34,265	20,394	31,356	23,832	31,319
123,872	193,425	134,924	184,424	139,684	173,694	146,228	146,892
372,824		374,137		365,128		348,271	

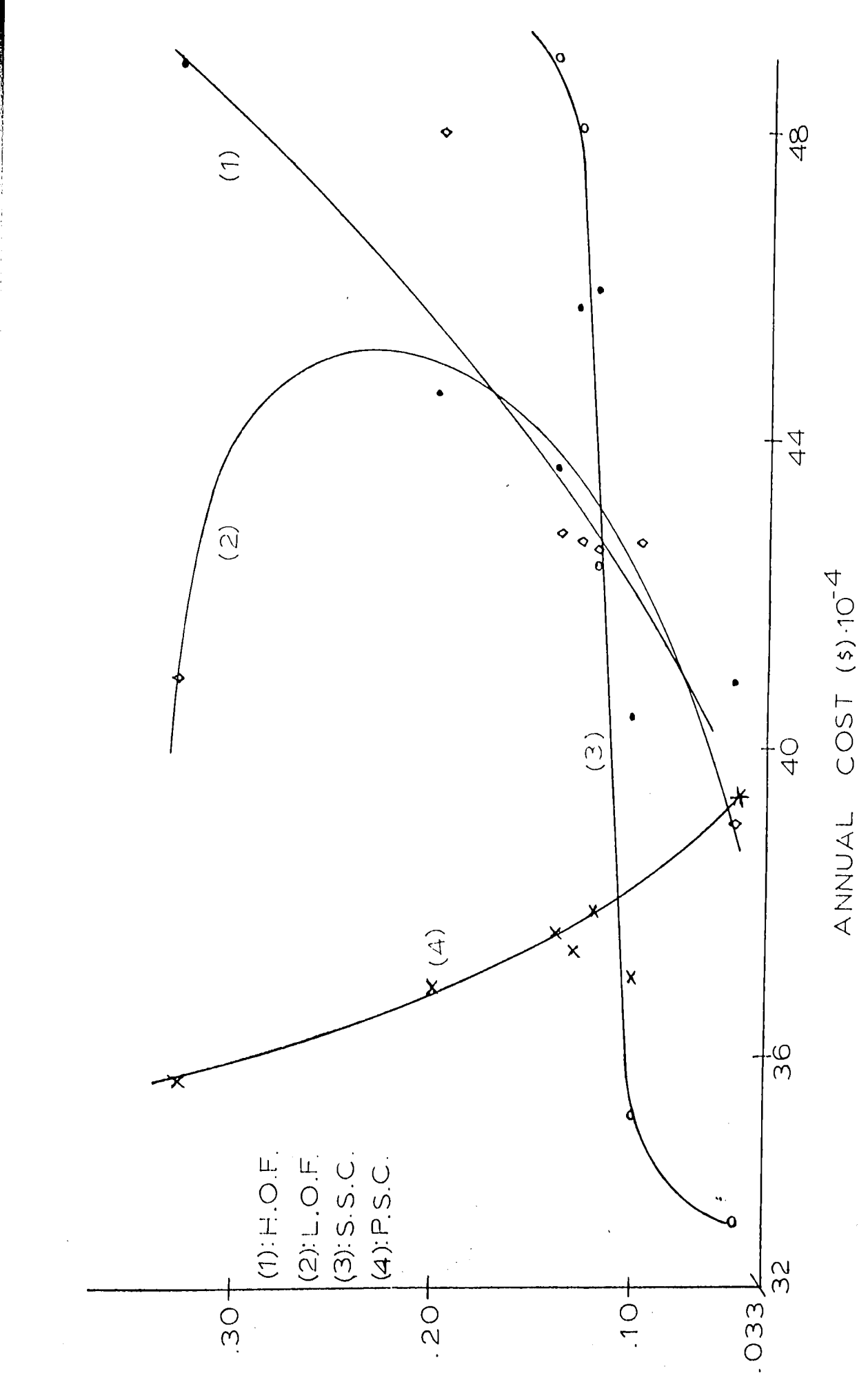

Figure 12.- Total annual cost for the four schemes tested

much benzene will come out in the sidestream. Therefore the column internal vapor rate must be raised approximately in direct proportion to the benzene concentration in the feed. This is what makes heat input increase rapidly with the increase in the concentration of benzene in the feed.

The H.O.F. and L.O.F. configurations are never the most economic ones for the examined cases.

For very low feed concentration of the lightest component, i.e., 5 percent of benzene, where the SSC configuration is the most economic one, we wanted to see how the results change for a system with relative volatilities not so large.

Therefore, we tested such a system having relative volatilities 1:2:3. Results are given in Table 7. The SSC configuration is again the most economic one but now the second best system in the L.O.F. What we observe though, is that the cost of the SSC configuration increased by about $ 120,000 compared with the cost for the higher relative volatilities column, with the same feed's composition, while the cost of the conventional system increased by about $ 80,000. Therefore, we cannot generalize the results that for low concentrations of the lightest component the SSC configuration is the most economic one, ignoring the relative volatilities. It is definitely the most economic when the relative volatilities are fairly large.

Table 7

Results for a system with relative volatilities 1:2:3, and for 5 percent of the volatile component at the feed.

Name of Configuration		L.O.F.		S.S.C.	P.S.C.	
# of column		1	2		1	2
$Q *10^{-6}$	Btu/hr	5.7	11.5	15.0	8.01	11.65
A_D	Sqft	318.3	561	857	401.6	653.2
Q_B*10-6	Btu/hr	5.7	12.0	15.5	8.13	11.8
A_R	Sqft	1,072	2,041	2,716	1,905	2,059
NT		37	22	46	21	48
NF		11	11	24	7	39/25
NS		-	-	29	-	29
RR		29.2	1.85	80.2	2.12	60.9
Diameter	inches	73	99.5	120.8	83.4	105.4
T_B	°F	315	346	346	328.5	346
T_D	°F	268	294	268	289.5	268
Fixed charges on equipment	$	31,060	34,815	78,256	26,949	68,520
Steam and cooling water	$	120,903	281,094	374,261	172,074	283,749
Annual cost of system	$	467,872		452,517	551,292	

APPENDIX A

NOMENCLATURE

NT	Total number of trays
NF	Feed tray
NS	Sidestream tray
J	Number of components
L(N)	Liquid flow from a tray (N)
V(N)	Vapor flow from a tray
X(N,J)	Liquid composition of a component (J) on a tray (N)
Y(N,T)	Vapor composition of a component (J) above a tray (N)
BOT	Bottom flowrate
XB(J)	Bottom's composition of a component (J)
TB	Reboiler's temperature
Q_B	Heat input
V_B	Vapor boilup
YB(J)	Vapor composition of a component (J) in reboiler
A_R	Reboiler's area
R	Reflux flowrate
RR	Reflux ratio
DIST	Distillate's flowrate
XD(J)	Distillate's composition of a component (J)
T_D	Distillate's temperature
Q_D	Condenser's duty
A_D	Condenser's area

TF	Feed's temperature
T(N)	Temperature on a tray (N)
LS	Sidestream's flowrate
XS(J)	Sidestream's composition of a component (J)
HL(N)	Liquid enthalpy on a tray (N)
HV(N)	Vaport enthalpy above a tray (N)
HL(R)	Reflux enthalpy
HVB	Vapor's boilup enthalpy
HLB	Bottom's product enthalpy
HLF	Liquid feed flowrate enthalpy
HVF	Vapor feed flowrate enthalpy
FL	Liquid feed flowrate
FV	Vapor feed flowrate
TBP	Bubble point temperature for feed
TDP	Dew point temperature for feed
K(N,T)	K-value of a component (J) on a tray (N)

The number 1 after these symbols stands for the first Distillation column, i.e., X1(N,J), while 2 stands for the second one, i.e., X2(N,J)

The temperatures are in °F, the areas in sq-ft, the flow rates in lbmole/hr, the concentrations in mole fractions, the heat input in Btu/hr and the enthalpies in Btu/lb-mole.

APPENDIX B

PHYSICAL PROPERTIES

The data was taken from the Technical Data Book - Petroleum Refining (1970), and was curvefitted by LEAPS.

K-Values

$$K(J) = A(J) + B(J) * T + C(J) * T^2 + D(J) * T^3$$

A(J)	B(J)
-3.265622173592163	.04158677712303
-1.019536199426184	.014404970304792
-.196787330257926	.004240024558143

C(J)	D(J)
-.000179660123307	.000000340424969
-.000072247077043	.000000158470271
-.000029042912739	.000000076307851

The above values are correct under the assumption of ideal vapor-liquid equilibrium.

Vapor Enthalpy in Btu/lbmole

$$HV(J)=HVCNST(1,J)+HVCNST(2,J)*T+HVCNST(3,J)*T^2$$

HVCNST(1,J)	HVCNST(2,J)	HVCNST(3,J)
20037.00437500	18.8809643	.0155327
22878.9817647	23.7321880	.0188310
26628.9693015	30.3378785	.0210486

$$HV_{total} = \sum_J HV(J)*Y(J)$$

Liquid Enthalpy in Btu/lbmole

$$HL(J)+HLCNJT(1,J)+HLCNST(2,J)*T+HLCNST(3,J)*T^2$$

HLCNST(1,J)	HLCNST(2,J)	HLCNST(3,J)
4516.1220622	30.4092456	.0240791
5590.7386765	34.5672659	.0282023
7023.4962868	40.7413760	.0292636

$$HL_{total} = \sum_J HL(J)*X(J)$$

APPENDIX C

DIGITAL PROGRAM DESCRIPTION AND LISTING

The program operates in the following way when given information on number of plates, feed plates, sidestream plate location, products' and feed's flowrates, feed's compositions, and products specifications.

(1) Routine CLMN is called to establish the steady state profile, for a conventional column and a given RR.

(2) If the products' composition is not the desired one, RR changes and routine CLMN is called again.

(3) When the products are the desired ones, routine CLMN1 is called to establish the steady state profile for a sidestream column.

(4) The procedure in step 2 is followed again and routine CLMN1 is re-called.

(5) Final results for both columns are printed.

PROGRAM DESCRIPTION

```
C.....................................................................
CCC
CCC     STEADYSTATE MULTICOMPONENT EXAMPLE USING WANG-HENKE
CCC     SYSTEM OF TWO DISTILLATION COLUMNS,WHERE THE TOP AND
CCC     BOTTOM PRODUCTS OF THE FIRST ARE FEEDS OF THE SECOND.
CCC     THE SECOND COLUMN HAS A LIQUID SIDESTREAM DRAW-OFF
CCC     SYSTEM: BENZENE ,TOLUENE ,O-XYLENE
CCC     THIS PROGRAM SIMULATES THE CASE WHERE WE HAVE FIXED
CCC     FLOWRATES AND SPECIFIED DISTILLATE COMPOSITION FOR THE
CCC     HEAVY COMPONENT OF THE FIRST COLUMN,AND BOTTOM COMPOSITION
CCC     FOR THE LIGHT COMPONENT OF THE SECOND.
CCC     WE ACHIEVE THE WANTED STEADY-STATE BY VARYING THE REFLUX RATIO.
CCC     WE ASSUME TOTAL CONDENSER AND PARTIAL REBOILER,AND THAT THE
CCC     FEEDS ARE SATURATED LIQUIDS.
CCC     AT THIS PROGRAM:
CCC                       1   STANDS FOR  BENZENE
CCC                       2   STANDS FOR  TOLUENE
CCC                       3   STANDS FOR  O-XYLENE
C.....................................................................
      DIMENSION X1(50,5),X2(50,5),Y1(50,5),Y2(50,5),KF(5),XB1(5),
     1XB2(5),YB1(5),YB2(5),XD1(5),XD2(5),YD1(5),YD2(5),L1(50),L2(50),
     2V1(50),V2(50),T1(50),T2(50),XF1(5),YF1(5),ZF1(5),XF2(5),YF2(5),
     3Y(5),X(5),ZF2(5),KB1(5),KB2(5),KD1(5),KD2(5),K1(50,5),K2(50,5),
     4XF3(5),ZF3(5),XF4(5),YF4(5),YF3(5)
      COMMON NJ
      REAL L1,KF,K1,KB1,KD1,LS2,L2,K2,KB2,KD2,LS1
      INTEGER S
      ZF1(1)=.05    $    ZF1(2)=.475    $    ZF1(3)=.475
      NT1=21    $    NF1=7    $    NJ=3
      DIST1=194.85    $    BOT1=405.15
      DIST2=15.79    $    BOT2=284.21
      TF1=304.56    $    F1=600.    $    RR1=2.1240    $    RR2=60.914
      NT2=48    $    NF2=25    $    NF3=39    $    NS2=29
      PRINT 500
      PRINT 501,(ZF1(J),J=1,NJ)
      S=1

CCC   BUBBLE POINT CALCULATIONS

      TB1=TF1
      CALL EQUIL(ZF1,Y,S,TB1)
      TBP=TB1
      TF1=TBP
      PRINT 502,(Y(J),J=1,NJ),TBP

CCC   DEW POINT CALCULATIONS

      S=2
      CALL EQUIL(X,ZF1,S,TB1)
      TDP=TB1
      PRINT 503,(ZF1(J),J=1,NJ)
      PRINT 504,(X(J),J=1,NJ),TDP
      IF(TF1 .GT. TBP) GO TO 101
      FV1=0.
      DO 1 J=1,NJ
      YF1(J)=0.
 1    XF1(J)=ZF1(J)
      GO TO 102
101   IF(TF1 .LT. TDP) GO TO 103
      FL1=0.
      DO 2 J=1,NJ
      XF1(J)=0.
 2    YF1(J)=ZF1(J)
      FV1=F1-FL1
      GO TO 105

CCC   ISOTHERMAL FLASH

103   FV1=.6*F1
      PRINT 505,(ZF1(J),J=1,NJ),TF1
      CALL ISOFL(XF1,YF1,ZF1,F1,K,FV1,TF1)
      PRINT 506, (XF1(J),J=1,NJ),(YF1(J),J=1,NJ)
102   FL1=F1-FV1
105   CONTINUE

CCC                       FIRST COLUMN
```

```
      PRINT 550
      M=0
      DR=.0005
      FLAGM=-1
      FLAGP=-1
  110 CALL CLMN(XB1,YB1,KB1,XD1,YD1,KD1,X1,Y1,K1,TB1,TD1,T1,L1,V1,RR1,
     1DIST1,BOT1,R1,XF1,YF1,NT1,NF1,F1,QB1,QD1,FV1,FL1,M,LOOP1,ZF1,TF1,
     2VB1)
      PRINT 508,LOOP1,RR1,R1,(XB1(J),J=1,NJ),BOT1,(XD1(J),J=1,NJ),DIST1
      IF (ABS(XD1(3)-.005) .LT. .00000001) GO TO 106
C
C     CHANGE THE REFLUX RATIO,USING THE INTERVAL HALVING METHOD,TO
C     ACHIEVE THE DESIRED OVERHEAD COMPOSITION.
C
      IF(XD1(3)-.005) 107,106,108
  107 IF (FLAGM .LT. 0) GO TO 109
      DR=DR/2.
  109 RR1=RR1-DR
      FLAGP=1
      GO TO 110
  108 IF(FLAGP .LT. 0) GO TO 111
      DR=DR/2.
  111 RR1=RR1+DR
      FLAGM=1
      GO TO 110
C
C             SECOND COLUMN
C
  106 TF2=TD1
      TF3=TB1
C
C     DISTILLATES PHASE CONDITION:VAPOR
C     BOTTOM'S PHASE CONDITION : LIQUID
C     CONDITION OF FEEDS OF THE SECOND COLUMN : SATURATED LIQUIDS
C
      FV2=0.
      F2=DIST1
      FL2=DIST1
      FV3=0.
      F3=BOT1
      FL3=BOT1
      DO 4 J=1,NJ
      XF2(J)=XD1(J)
      YF2(J)=0.
      XF3(J)=XB1(J)
      YF3(J)=0.
    4 ZF2(J)=ZF1(J)
      LS2=F1-BOT2-DIST2
      I=0
      DR=.0005
      FLAGM=-1
      FLAGP=-1
      PRINT 560
  150 CALL CLMN1(XB2,YB2,KB2,XD2,YD2,KD2,X2,Y2,K2,TB2,TD2,T2,L2,V2,RR2,
     1DIST2,BOT2,R2,XF2,YF2,NT2,NF3,F2,QB2,QD2,FV2,FL2,I,LOOP,ZF2,TF2,
     2VB2,XF3,YF3,FV3,FL3,TF3,LS2,NS2,F3,NF2)
      PRINT 511,LOOP,RR2,R2,(XB2(J),J=1,NJ),BOT2,(XD2(J),J=1,NJ),DIST2,
     1(X2(NS2,J),J=1,NJ),LS2
      IF (ABS(XB2(2)-.05) .LT. .00000001) GO TO 130
C
C     CHANGE THE REFLUX RATIO,USING THE INTERVAL HALVING METHOD,TO
C     ACHIEVE THE DESIRED BOTTOM COMPOSITION.
C
      IF(XB2(2)-.05) 117,130,118
  117 IF (FLAGM .LT. 0) GO TO 119
      DR=DR/2.
  119 RR2=RR2-DR
      FLAGP=1
      GO TO 150
  118 IF(FLAGP .LT. 0) GO TO 121
      DR=DR/2.
  121 RR2=RR2+DR
      FLAGM=1
      GO TO 150
  130 CONTINUE
C
C     PRINT FINAL RESULTS FOR BOTH COLUMNS
C
      PRINT 512
```

```
      PRINT 509
      NN=0
      TF4=0.
      FL4=0.
      FV4=0.
      LS1=0.
      NS1=0.
      NF4=0.
      DO 9 J=1,NJ
      XF4(J)=0.
    9 YF4(J)=0.
      CALL SPRINT(M,LOOP1,NT1,NF1,XF1,FV1,YF1,FL1,TB1,XB1,YB1,VB1,
     1X1,T1,Y1,V1,L1,TD1,XD1,YD1,R1,DIST1,BOT1,RR1,QB1,QD1,TF1,NN,
     2LS1,NS1,XF4,YF4,NF4,FV4,FL4,TF4)
      VMAX=0.
      DO 358 N=1,NT1
      V=V1(N)
  358 VMAX=AMAX1(VMAX,V)
      CALL CLMSP(ZF1,TB1,TD1,VMAX,QD1,QB1)
      PRINT 19
      NN=1
      CALL SPRINT(I,LOOP,NT2,NF3,XF2,FV2,YF2,FL2,TB2,XB2,YB2,VB2,
     1X2,T2,Y2,V2,L2,TD2,XD2,YD2,R2,DIST2,BOT2,RR2,QB2,QD2,TF2,NN,LS2,
     2NS2,XF3,YF3,NF2,FV3,FL3,TF3)
      VMAX=0.
      DO 359 N=1,NT2
      V=V2(N)
  359 VMAX=AMAX1(VMAX,V)
      CALL CLMSP(ZF1,TB2,TD2,VMAX,QD2,QB2)
  500 FORMAT(///,30X,*BUBBLE POINT CALCULATION*)
  501 FORMAT(/,1X,*X(1)=*,E15.5,5X,*X(2)=*,E15.5,5X,*X(3)=*,E15.5,5X)
  502 FORMAT(/,1X,*Y(1)=*,E15.5,5X,*Y(2)=*,E15.5,5X,*Y(3)=*,E15.5,5X,
     1*TBP=BUBBLE POINT TEMPERATURE=*,E10.4)
  503 FORMAT(///,30X,*DEW POINT CALCULATION*,/1X,*Y(1)=*,E15.5,5X,
     1*Y(2)=*,E15.5,5X,*Y(3)=*,E15.5)
  504 FORMAT(/,1X,*X(1)=*,E15.5,10X,*X(2)=*,E15.5,10X,*X(3)=*,E15.5,10X,
     1*TDP=DEW POINT TEMPERATURE=*,E10.4)
  505 FORMAT(///,25X,*ISOTHERMAL FLASH CALCULATION*,/,1X,*Z(1)=*,E15.5,
     15X,*Z(2)=*,E15.5,5X,*Z(3)=*,E15.5,5X,*TF1=*,E15.5)
  506 FORMAT(/,1X,*X(1)=*,E15.5,5X,*X(2)=*,E15.5,5X,*X(3)=*,E15.5,/,
     11X,*Y(1)=*,E15.5,5X,*Y(2)=*,E15.5,5X,*Y(3)=*,E15.5)
  508 FORMAT(///,1X,*ITERATION NO=*,I4,10X,*RR=*,F6.3,10X,*R=*,F10.5,
     1//,1X,*XB(1)=*,E15.5,10X,*XB(2)=*,E15.5,10X,*XB(3)=*,E15.5,,10X,
     2*BOT=*,F7.3,/,1X,*XD(1)=*,E15.5,10X,*XD(2)=*,E15.5,10X,*XD(3)=*,
     3E15.5,10X,*DIST=*,F7.3)
  511 FORMAT(///,1X,*ITERATION NO=*,I4,10X,*RR=*,F6.3,10X,*R=*,F10.5,
     1//,1X,*XB(1)=*,E15.5,10X,*XB(2)=*,E15.5,10X,*XB(3)=*,E15.5,,10X,
     2*BOT=*,F7.3,/,1X,*XD(1)=*,E15.5,10X,*XD(2)=*,E15.5,10X,*XD(3)=*,
     3E15.5,10X,*DIST=*,F7.3//1X,*XS1(1)=*,E15.5,10X,*XS1(2)=*,E15.5,
     410X,*XS1(3)=*,E15.5,10X,*LS1=*,F7.3/)
  550 FORMAT(///,30X,*INTERMEDIATE RESULTS FOR FIRST COLUMN*)
  560 FORMAT(///,30X,*INTERMEDIATE RESULTS FOR SECOND COLUMN*)
  512 FORMAT(///,60X,*FINAL RESULTS*/55X,*.....*)
  509 FORMAT(///,63X,*FIRST COLUMN*)
   19 FORMAT(//50X,*.....*//50X,* DISTILLAT
     1ION COLUMN WITH LIQUID SIDESTREAM*//
     350X,*.....*)
      STOP
      END



      SUBROUTINE CLMN(XB,YB,KB,XD,YD,KD,X,Y,K,TB,TD,T,L,V,RR,DIST,
     1BOT,R,XF,YF,NT,NF,F,QB,QD,FV,FL,I,LOOP,ZF,TF,VB)
C.....
CCC
CCC     SUBROUTINE CLMN COMPUTES THE STEADY-STATE FOR A GIVEN RR,
CCC     FOR A CONVENTIONAL COLUMN,WHEN GIVEN INFORMATION ON FEED
CCC     AND DESIRED FLOWRATES.
CCC     IT USES THE WANG-HENKE METHOD FOR CONVERSION,WITH THE
CCC     DIFFERENCE THAT INSTEAD OF USING SUCCESSIVE SUBSTITUTION,
CCC     IT USES THE SINGLE THETA METHOD TO COMPUTE NEW X*S,BASED ON
CCC     THE X*S THAT COME FROM THE TRIDIAGONAL MATRIX.
CCC
C.....
      DIMENSION X(50,5),Y(50,5),K(50,5),XB(5),KB(5),YB(5),XD(5),YD(5),
     1KD(5),L(50),V(50),XX(51),KK(5),YY(5),T(50),XF(5),YF(5),HL(50),
     2HV(50),A(51),B(51),C(51),D(51),ZF(5),TOLD(50),OLBXBD(5),NEWXD(5),
     3XBOLD(5),XOLD(50,5),XDOLD(5),E(5),G(5),H(5),U(5)
```

```
      COMMON NJ
      REAL K,KK,KB,KD,L,NEWXD
      INTEGER S
      E(1)=-3.2656221735921635    $   E(2)=-1.019536199426184
      E(3)=-.1967873302579 26
      G(1)=.04158677121303    $   G(2)=.01440497030479 2
      G(3)=.00424002455814 3
      H(1)=-.00017966012330 7    $   H(2)=-.00007224707704 3
      H(3)=-.00002904291273 9
      U(1)=.00000034042496 9    $   U(2)=.00000015847027 1
      U(3)=.00000007630785 1
      S=1
      R=RR*DIST
      I=I+1
      LOOP=0
C
CC    GUESS INITIAL TEMPERATURUS AND FLOWS
C
      TB=TF+40.
      TBOLD=TB
      TD=TF-40.
      TDOLD=TD
      VB=R+DIST
      DT=(TB-TD)/(NT+1)
      DO 1 N=1,NT
      XN=FLOAT(N)
      T(N)=TB-XN*DT
      TOLD(N)=T(N)
      V(N)=VB
      IF(N .GT. NF) V(N)=VB+FV
      L(N)=R
      IF(N .LE. NF) L(N)=R+FL
    1 CONTINUE
      CALL ENTH(XF,YF,TF,HLF,HVF)
  100 LOOP=LOOP+1
      DO 31 J=1,NJ
   31 KB(J)=E(J)+G(J)*TB+H(J)*TB*TB+U(J)*TB*TB*TB
      DO 30 N=1,NT
      DO 35 J=1,NJ
   35 K(N,J)=E(J)+G(J)*T(N)+H(J)*T(N)*T(N)+U(J)*T(N)*T(N)*T(N)
   30 CONTINUE
C
CC    CALCULATE TRIDIAGONAL MATRIX FOR EACH COMPONENT
C
      DO 2 J=1,NJ
      A(1)=-BOT-VB*KB(J)
      B(1)=L(1)
      D(1)=0.
      A(2)=-L(1)-V(1)*K(1,J)
      B(2)=L(2)
      C(2)=KB(J)*VB
      D(2)=0.
      NTM1=NT-1
      DO 3 N=2,NTM1
      A(N+1)=-L(N)-V(N)*K(N,J)
      B(N+1)=L(N+1)
      C(N+1)=K(N-1,J)*V(N-1)
      D(N+1)=0.
      NFP1=NF+1
      IF(N .EQ. NFP1) D(NF+2)=-FV*YF(J)
      IF(N .EQ. NF)  D(NF+1)=-FL*XF(J)
    3 CONTINUE
      A(NT+1)=R*K(NT,J)-V(NT)*K(NT,J)-L(NT)
      C(NT+1)=K(NT-1,J)*V(NT-1)
      D(NT+1)=0.
C
CC    SOLVE FOR NEW X
C
      CALL TRIDI(A,B,C,D,NT+1,XX)
      XB(J)=XX(1)
      XBOLD(J)=XB(J)
      DO 4 N=1,NT
      X(N,J)=XX(N+1)
    4 XOLD(N,J)=X(N,J)
    2 CONTINUE
      DO 14 J=1,NJ
      Y(NT,J)=K(NT,J)*X(NT,J)
      XD(J)=Y(NT,J)
   14 XDOLD(J)=XD(J)
```

```
C
CCCCC     USE THETA METHOD FOR CONVERSION
CCCCCC
CCCCCC    TETA=W
CCCCCC    FOR A CONVENTIONAL COLUMN AND WHEN USING NEWTON-RAPHSON
C         METHOD,THE INITIAL VALUE OF THETA IS ALWAYS ZERO.
C
          W=0.
C
CCC       OLDXBD(J)=XB(J)/XD(J) FROM TRIDIAGONAL
C
  112     SUMNXD=0.
          DO 5 J=1,NJ
          OLDXBD(J)=XB(J)/XD(J)
**********************
          NEWXD(J)=F*ZF(J)/((1.+W*(BOT/DIST)*OLDXBD(J))*DIST)
    5     SUMNXD=SUMNXD+NEWXD(J)
          IF(ABS(SUMNXD-1.) .LT. .0000001) GO TO 110
          FNR=SUMNXD-1.
C
CCC       CALCULATE DERIVATIVES
C
          FNRSL=0.
          DO 6 J=1,NJ
    6     FNRSL=FNRSL-(NEWXD(J)*(BOT/DIST)*OLDXBD(J))/(1.+W*(BOT/DIST)*
         1OLDXBD(J))
C
CCC       CALCULATE NEW THETA
C
          W=W-FNR/FNRSL
          GO TO 112
C
CCC       CALCULATE NEW X
C
  110     DO 7 J=1,NJ
          XD(J)=NEWXD(J)
    7     XB(J)=W*OLDXBD(J)*XD(J)
          XB1=0.
          DO 8 J=1,NJ
    8     XB1=XB1+XB(J)
          DO 9 J=1,NJ
    9     XB(J)=XB(J)/XB1
          DO 10 N=1,NT
          XSUM=0.
          DO 11 J=1,NJ
   11     XSUM=(XOLD(N,J)/XDOLD(J))*XD(J)+XSUM
          DO 12 J=1,NJ
   12     X(N,J)=((XOLD(N,J)/XDOLD(J))*XD(J))/XSUM
   10     CONTINUE
C
CCC       CALCULATE NEW TEMPERATURES,Y AND ENTHALPIES
C
          CALL EQUIL(XB,YB,S,TB)
          CALL ENTH(XB,YB,TB,HLB,HVB)
          TSUM=ABS(TB-TBOLD)
          TBOLD=TB
          DO 15 N=1,NT
          DO 16 J=1,NJ
   16     XX(J)=X(N,J)
          CALL EQUIL(XX,YY,S,T(N))
          DO 17 J=1,NJ
   17     Y(N,J)=YY(J)
          CALL ENTH(XX,YY,T(N),HL(N),HV(N))
          TSUM=TSUM+ABS(T(N)-TOLD(N))
          TOLD(N)=T(N)
   15     CONTINUE
          DO 18 J=1,NJ
   18     XD(J)=Y(NT,J)
          CALL EQUIL(XD,YD,S,TD)
          CALL ENTH(XD,YD,TD,HLR,HVR)
          TSUM=TSUM+ABS(TD-TDOLD)
          TDOLD=TD
C
          CALCULATE REBOILER AND CONDENSER DUTIES
C
          QD=V(NT)*HV(NT)-(R+DIST)*HLR
          QB=L(1)*HL(1)-VB*HVB-BOT*HLB
C
          CALCULATE NEW LIQUID AND VAPOR RATES
```

```
C
      V(NT)=R+DIST
      V(NT-1)=(V(NT)*HV(NT)-R*HLR-DIST*HL(NT))/(HV(NT-1)-HL(NT))
      L(NT)=V(NT-1)-DIST
      NR=NT-NF-2
      DO 19 N=1,NR
      NP=NT-N
      V(NP-1)=(V(NP)*(HV(NP)-HL(NP))-L(NP+1)*(HL(NP+1)-HL(NP)))/
     1(HV(NP-1)-HL(NP))
   19 L(NP)=L(NP+1)+V(NP-1)-V(NP)
      V(NF)=(FV*(HL(NF+1)-HVF)+L(NF+2)*(HL(NF+1)-HL(NF+2))
     1+V(NF+1)*(HV(NF+1)-HL(NF+1)))/(HV(NF)-HL(NF+1))
      L(NF+1)=L(NF+2)+V(NF)+FV-V(NF+1)
      V(NF-1)=(V(NF)*(HV(NF)-HL(NF))+L(NF+1)*(HL(NF)-HL(NF+1))
     1+FL*(HL(NF)-HLF))/(HV(NF-1)-HL(NF))
      L(NF)=L(NF+1)+V(NF-1)+FL-V(NF)
      NFM2=NF-2
      DO 20 N=1,NFM2
      NP=NF-N
      V(NP-1)=(V(NP)*(HV(NP)-HL(NP))-L(NP+1)*(HL(NP+1)-HL(NP)))/
     1(HV(NP-1)-HL(NP))
   20 L(NP)=L(NP+1)+V(NP-1)-V(NP)
      VB=(V(1)*(HV(1)-HL(1))+L(2)*(HL(1)-HL(2)))/(HVB-HL(1))
      L(1)=L(2)+VB-V(1)
      IF (TSUM .LE. .01) GO TO 120
      GO TO 130
  120 CONTINUE
      RETURN
      END

ARITHMETIC STATEMENT FUNCTION ERROR
50



      SUBROUTINE CLMN1(XB,YB,KB,XD,YD,KD,X,Y,K,TB,TD,T,L,V,RR,DIST,
     1BOT,R,XF1,YF1,NT,NF1,F1,QB,QD,FV1,FL1,I,LOOP,ZF,TF1,VB,XF2,YF2,
     2FV2,FL2,TF2,LS,NS,F2,NF2)
C.....................................................................
C
C     SUBROUTINE CLMN1 COMPUTES THE STEADY-STATE FOR ACOLUMN WITH
C     ASIDESTREAM DRAWOFF,WHEN GIVEN INFORMATION ON FEED,DESIRED
C     FLOWRATES AND REFLUX RATIO.
C     IT USES THE WANG-HENKE METHOD FOR CONVERSION WITH THE
C     DIFFERENCE THAT INSTEAD OF USING SUCCESSIVE SUBSTITUTION,
C     IT USES THE THETA METHOD(TWO THETAS  USED),TO COMPUTE NEW
C     X*S,BASED ON THE X*S THAT COME FROM THE TRIDIAGONAL MATRIX.
C
C.....................................................................
      DIMENSION X(50,5),Y(50,5),K(50,5),XB(5),KB(5),YB(5),XD(5),YD(5),
     1KD(5),L(50),V(50),XX(51),KK(5),YY(5),T(50),XF1(5),YF1(5),HL(50),
     2HV(50),A(51),B(51),C(51),D(51),ZF(5),TOLD(50),OLDXBD(5),NEWXD(5),
     6XBOLD(5),XOLD(50,5),XDOLD(5),E(5),G(5),H(5),U(5),OLDXLD(5),
     4OLDXBL(5),NEWX(50,5),F(50),FL(50),FV(50),LS1(50),LV1(50),HVF(50),
     5HLF(50),XF2(5),YF2(5)
      COMMON NJ
      REAL K,KK,KB,KD,L,NEWXD,NEWX,LS,LS1,LV1
      INTEGER S
      E(1)=-3.2656221735921635    $    E(2)=-1.019536199426184
      E(3)=-.196787330257926
      G(1)=.041586777121303    $    G(2)=.014404970304792
      G(3)=.0042400245581 43
      H(1)=-.000179660123307    $    H(2)=-.000072247077043
      H(3)=-.000029042912739
      U(1)=.000000340424969    $    U(2)=.000000158470271
      U(3)=.000000076307851
      S=1
      R=RR*DIST
      I=I+1
      LOOP=0

C     GUESS INITIAL TEMPERATURUS AND FLOWS

      TB=350.
      TBOLD=TB
      TD=270.
      TDOLD=TD
      VB=R+DIST
      DT=(TB-TD)/(NT+1)
```

```
      DO 1 N=1,NT
      XN=FLOAT(N)
      T(N)=TB-XN*DT
      TOLD(N)=T(N)
      V(N)=VB
      IF(N .GT. NF2) V(N)=VB+FV2
      IF(N .GT. NF1) V(N)=VB+FV1+FV2
      L(N)=R
      IF(N .LE. NF2) L(N)=R-LS+FL1+FL2
      IF (N .LT. NS .AND. N .GT. NF2) L(N)=R-LS+FL1
      IF(N .LE. NF1 .AND. N .GE. NS)L(N)=R+FL1
    1 CONTINUE
      CALL ENTH(XF1,YF1,TF1,HLF1,HVF1)
      CALL ENTH(XF2,YF2,TF2,HLF2,HVF2)
      DO 400 N=1,NT
      F(N)=0.
      FL(N)=0.
      FV(N)=0.
      LS1(N)=0.
      LV1(N)=0.
      HVF(N)=0.
      HLF(N)=0.
      IF (N .EQ. NS) LS1(N)=LS
      IF(N .EQ. NF1) GO TO 410
      IF(N .EQ. NF2) GO TO 430
      GO TO 420
  410 F(NF1)=F1
      FL(NF1)=FL1
      HVF(NF1)=HVF1
      HLF(NF1)=HLF1
      GO TO 420
  430 F(NF2)=F2
      FL(NF2)=FL2
      FV(NF2)=FV2
      HVF(NF2)=HVF2
      HLF(NF2)=HLF2
  420 CONTINUE
  400 CONTINUE
  130 LOOP=LOOP+1
      DO 31 J=1,NJ
   31 KB(J)=E(J)+G(J)*TB+H(J)*TB*TB+U(J)*TB*TB*TB
      DO 30 N=1,NT
      DO 35 J=1,NJ
   35 K(N,J)=E(J)+G(J)*T(N)+H(J)*T(N)*T(N)+U(J)*T(N)*T(N)*T(N)
   30 CONTINUE

      CALCULATE TRIDIAGONAL MATRIX FOR EACH COMPONENT

      DO 2 J=1,NJ
      A(1)=-BOT-VB*KB(J)
      B(1)=L(1)
      D(1)=0.
      A(2)=-L(1)-VT1)*K(1,J)
      B(2)=L(2)
      C(2)=KB(J)*VB
      D(2)=0.
      NTM1=NT-1
      DO 3 N=2,NTM1
      A(N+1)=-L(N)-V(N)*K(N,J)
      B(N+1)=L(N+1)
      C(N+1)=K(N-1,J)*V(N-1)
      D(N+1)=0.
      NFP1=NF1+1
      IF(N .EQ. NFP1) D(NF1+2)=-FV1*YF1(J)
      IF(N .EQ. NF1)  D(NF1+1)=-FL1*XF1(J)
      NF2P1=NF2+1
      IF(N .EQ. NF2P1) D(NF2+2)=-FV2*YF2(J)
      IF(N .EQ. NF2) D(NF2+1)=-FL2*XF2(J)
      NSM1=NS-1
      IF(N .EQ. NSM1) B(N+1)=L(N+1)-LS
    3 CONTINUE
      A(NT+1)=R*K(NT,J)-V(NT)*K(NT,J)-L(NT)
      C(NT+1)=K(NT-1,J)*V(NT-1)
      D(NT+1)=0.

      SOLVE FOR NEW X

      CALL TRIDI(A,B,C,D,NT+1,XX)
      XB(J)=XX(1)
```

```
      XBOLD(J)=XB(J)
      DO 4 N=1,NT
      X(N,J)=XX(N+1)
    4 XOLD(N,J)=X(N,J)
    2 CONTINUE
      DO 14 J=1,NJ
      Y(NT,J)=K(NT,J)*X(NT,J)
      XD(J)=Y(NT,J)
   14 XDOLD(J)=XD(J)
C
C     USE THETA METHOD FOR CONVERSION
C
      THETA1=W1
      THETA2=W2
C     THE INITIAL VALUES OF THETAS SHOULD BE ONE(1),FOR THE METHOD
C     TO CONVERGE WHEN USING NEWTON-RAPHSON METHOD.
C
      FT=F1+F2
      W1=1.
      W2=1.
      OLDW1=W1
      OLDW2=W2
C
C     OLDXBD(J)=XB(J)/XD(J)   FROM TRIDIAGONAL
C     OLDXLD(J)=X(NS,J)/XD(J) FROM TRIDIAGONAL
C     OLDXBL(J)=XB(J)/X(NS,J)   FROM TRIDIAGONAL
C
  112 SUMNXD=0.
      SUMNXL=0.
      DO 5 J=1,NJ
      OLDXBD(J)=XB(J)/XD(J)
      OLDXLD(J)=X(NS,J)/XD(J)
      OLDXBL(J)=XB(J)/X(NS,J)
      NEWXD(J)=FT*ZF(J)/((1.+W1*(BOT/DIST)*OLDXBD(J)+W2*(LS/DIST)*
     1OLDXLD(J))*DIST)
      NEWX(NS,J)=W2*OLDXLD(J)*NEWXD(J)
      SUMNXL=SUMNXL+NEWX(NS,J)
    5 SUMNXD=SUMNXD+NEWXD(J)
      FNR1=SUMNXD-1.
      FNR2=SUMNXL-1.
      IF(ABS(FNR1) .LT. .00001 .AND. ABS(FNR2) .LT. .00001)GO TO 110
C
C     CALCULATE THE JACOBIAN OF OUR TWO FUNCTIONS FNR1,FNR2,BY
C     CALCULATING THE DERIVATIVES OF THOSE FUNCTIONS WITH
C     RESPECT TO W1,AND W2.
C
      DF1DW1=0.
      DF1DW2=0.
      DF2DW1=0.
      DF2DW2=0.
      DO 150  J=1,NJ
      DF1DW1=DF1DW1-(NEWXD(J)**2)*BOT*OLDXBD(J)/(FT*ZF(J))
      DF1DW2=DF1DW2-(NEWXD(J)**2)*LS*OLDXLD(J)/(FT*ZF(J))
      DF2DW1=DF2DW1-(NEWX(NS,J)**2)*BOT*OLDXBL(J)/(FT*ZF(J)*W2)
  150 DF2DW2=DF2DW2+(NEWX(NS,J)**2)*(W1*BOT*OLDXBL(J)+LS/((LS/DIST)*
     1OLDXLD(J)))/((FT*ZF(J))*(W2**2))
      Q=DF1DW1*DF2DW2-DF1DW2*DF2DW1
C
C     FIND THE CHANGE IN THETAS
C
      DW1=(FNR2*DF1DW2-FNR1*DF2DW2)/Q
      DW2=(FNR1*DF2DW1-FNR2*DF1DW1)/Q
C
C     CALCULATE NEW THETAS
C
      W1=W1+DW1
      W2=W2+DW2
      IF (W1 .LT. 0.) W1=OLDW1/2.
      IF (W2 .LT. 0.) W2=OLDW2/2.
      OLDW1=W1
      OLDW2=W2
      GO TO 112
C
C     CALCULATE NEW X
C
  110 DO 7 J=1,NJ
      XD(J)=NEWXD(J)
    7 XB(J)=W1*OLDXBD(J)*XD(J)
      DO 270 N=1,NT
```

```
      X2SUM=0.
      DO 295 J=1,NJ
  295 X2SUM=X2SUM+XOLD(N,J)/XDOLD(J)*XD(J)
      DO 265 J=1,NJ
  265 X(N,J)=XOLD(N,J)/XDOLD(J)*XD(J)/X2SUM
  270 CONTINUE

      CALCULATE NEW TEMPERATURES,Y AND ENTHALPIES

      CALL EQUIL(XB,YB,S,TB)
      CALL ENTH(XB,YB,TB,HLB,HVB)
      TSUM=ABS(TB-TBOLD)
      TBOLD=TB
      DO 15 N=1,NT
      DO 16 J=1,NJ
   16 XX(J)=X(N,J)
      CALL EQUIL(XX,YY,S,T(N))
      DO 17 J=1,NJ
   17 Y(N,J)=YY(J)
      CALL ENTH(XX,YY,T(N),HL(N),HV(N))
      TSUM=TSUM+ABS(T(N)-TOLD(N))
      TOLD(N)=T(N)
   15 CONTINUE
      DO 18 J=1,NJ
   18 XD(J)=Y(NT,J)
      CALL EQUIL(XD,YD,S,TD)
      CALL ENTH(XD,YD,TD,HLR,HVR)
      TSUM=TSUM+ABS(TD-TDOLD)
      TDOLD=TD

      CALCULATE REBOILER AND CONDENSER DUTIES
      QD=V(NT)*HV(NT)-(R+DIST)*HLR

      QB=L(1)*HL(1)-VB*HVB-BOT*HLB

      CALCULATE NEW LIQUID AND VAPOR RATES

      V(NT)=R+DIST
      V(NT-1)=(V(NT)*HV(NT)-R*HLR-DIST*HL(NT))/(HV(NT-1)-HL(NT))
      L(NT)=V(NT-1)-DIST
      SUM1=0.
      NM2=NT-2
      DO 19 N=1,NM2
      NP=NT-N
      SUM2=SUM1
      SUM1=SUM1+F(NP)-LV1(NP)-LS1(NP)
      V(NP-1)=((V(NP)+SUM2-DIST)*HL(NP+1)-(V(NP)+LV1(NP))*HV(NP)
     1-(SUM1+LS1(NP)-DIST)*HL(NP)+FV(NP-1)*HVF(NP-1)+FL(NP)*HLF(NP))
     3/(HL(NP)-HV(NP-1))
      L(NP)=V(NP-1)+SUM1-DIST
   19 CONTINUE
      VB=(V(1)*(HV(1)-HL(1))+L(2)*(HL(1)-HL(2)))/(HVB-HL(1))
      L(1)=L(2)+VB-V(1)
      IF (TSUM .LE. .01) GO TO 120
      GO TO 130
  120 CONTINUE
      RETURN
      END


      SUBROUTINE EQUIL(X,Y,S,T)
C.....................................................................

      SUBROUTINE EQUIL PERFORMS BUBBLE-POINT AND DEW-POINT
      CALCULATIONS THROUGH NEWTON-RAPHSON ITERATIONS.
      THE K-VALUES OF THE COMPONENTS HAVE BEEN CURVFITTED WITH
      A THIRD DEGREE POLYNOMIAL.
      A,B,C,D, COEFFICIENTS OF K

C.....................................................................
      DIMENSION X(5),Y(5),K(5),A(5),B(5),C(5),D(5),E(5)
      COMMON NJ
      INTEGER S
      REAL K
      A(1)=-3.2656221735921635    $   A(2)=-1.019536199426184
      A(3)=-.196787330257926
      B(1)=.041586777121303    $    B(2)=.014404970304792
      B(3)=.004240024558143
```

```
      C(1)=-.0001796601233O7    $   C(2)=-.000072247077043
      C(3)=-.000029042912739
      D(1)=.000000340424969     $   D(2)=.000000158470271
      D(3)=.000000076307851
      IF(S .EQ. 2) GO TO 1
C
CC    BUBBLE-POINT CALCULATIONS
C
      ASUM=0.
      BSUM=0.
      CSUM=0.
      DSUM=0.
      DO 5 J=1,NJ
      ASUM=ASUM+A(J)*X(J)
      BSUM=BSUM+B(J)*X(J)
      CSUM=CSUM+C(J)*X(J)
    5 DSUM=DSUM+C(J)*X(J)
   20 SUM=ASUM+BSUM*T+CSUM*T*T+DSUM*T*T*T
      IF(ABS(SUM-1.) .LT. .0000001) GO TO 10
      FNR=SUM-1.
      FNRSL=BSUM+2*CSUM*T+3*DSUM*T*T
      T=T-FNR/FNRSL
      GO TO 20
   10 CONTINUE
      DO 30 J=1,NJ
      K(J)=A(J)+B(J)*T+C(J)*T*T+D(J)*T*T*T
   30 Y(J)=K(J)*X(J)
      RETURN
C
CC    DEW-POINT CALCULATIONS
C
    1 DO 2 J=1,NJ
      E(J)=A(J)+B(J)*T+C(J)*T*T+D(J)*T*T*T
    2 X(J)=Y(J)/E(J)
      XSUM=0.
      DO 3 J=1,NJ
    3 XSUM=XSUM+X(J)
      IF(ABS(XSUM-1.) .LT. .0000001) GO TO 40
      FNR=XSUM-1.
      FSLOPE=0.
      DO 4 J=1,NJ
    4 FSLOPE =FSLOPE+(-Y(J)*(B(J)+2*C(J)*T+3*D(J)*T*T)/(E(J)*E(J)))
      T=T-FNR/FSLOPE
      GO TO 1
   40 CONTINUE
      DO 60 J=1,NJ
      K(J)=A(J)+B(J)*T+C(J)*T*T+D(J)*T*T*T
   60 X(J)=Y(J)/K(J)
      RETURN
      END


      SUBROUTINE ENTH(X,Y,T,HL,HV)
C.....................................................................
C
C     SUBROUTINE ENTH COMPUTES THE ENTHALPIES FOR LIQUID(HL) AND
C     VAPOR (HV) IN BTU/LBMOLE.
C
C.....................................................................
      DIMENSION HLCNST(3,5),HVCNST(3,5),X(5),Y(5)
      COMMON NJ
      HLCNST(1,1)=4516.1220622 $ HLCNST(2,1)=30.4092456
      HLCNST(3,1)=.0240791
      HLCNST(1,2)=5590.7386765  $  HLCNST(2,2)=34.5672659
      HLCNST(3,2)=.0282023
      HLCNST(1,3)=7023.4962868   $   HLCNST(2,3)=40.7413760
      HLCNST(3,3)=.0292636
      HVCNST(1,1)=20037.0047500  $  HVCNST(2,1)=18.8809643
      HVCNST(3,1)=.0155327
      HVCNST(1,2)=22878.9817647  $  HVCNST(2,2)=23.7321880
      HVCNST(3,2)=.0188310
      HVCNST(1,3)=26628.9693015  $  HVCNST(2,3)=30.3378785
      HVCNST(3,3)=.0210486

      HL=HLCNST(1)+HLCNST(2)*T+HLCNST(3)*T*T
```

```
      HLSUM=0.
      HVSUM=0.
      DO 1 J=1,NJ
      HLSUM=HLSUM+(HLCNST(1,J)+HLCNST(2,J)*T+HLCNST(3,J)*T*T)*X(J)
    1 HVSUM=HVSUM+(HVCNST(1,J)+HVCNST(2,J)*T+HVCNST(3,J)*T*T)*Y(J)
      HL=HLSUM
      HV=HVSUM
      RETURN
      END


      SUBROUTINE TRIDI(A,B,C,D,N,X)
C.....................................................................
C
C     SUBROUTINE TRIDI SOLVES THE TRIDIAGONAL MATRIX FOR EACH
C     COMPONENT BY USING THE THOMAS METHOD
C
C.....................................................................
      DIMENSION A(51),B(51),C(51),D(51),X(51),W(51),G(51)
      W(1)=A(1)
      DO 5 J=2,N
    5 W(J)=A(J)-C(J)*B(J-1)/W(J-1)
      G(1)=D(1)/W(1)
      DO 10 J=2,N
   10 G(J)=(D(J)-C(J)*G(J-1))/W(J)
      X(N)=G(N)
      DO 15 J=2,N
      NC=N+1-J
   15 X(NC)=G(NC)-X(NC+1)*B(NC)/W(NC)
      RETURN
      END


      SUBROUTINE ISOFL(XF,YF,ZF,F,K,FV,TF)
C.....................................................................
C
C     SUBROUTINE ISOFL PERFORMS AN ISOTHERMAL FLASH CALCULATION,
C     WHEN CALLED FROM MAIN. IT ESTABLISHES THE VAPOR AND
C     LIQUID FLOWRATES,AS WELL AS THEIR COMPOTITION,OF A GIVEN
C     FEED,WHEN ITS TEMPERATURE IS BETWEEN ITS BUBBLE AND DEW
C     POINT TENPERATURES.
C
C.....................................................................
      DIMENSION XF(5),YF(5),ZF(5),K(5),A(5),B(5),C(5),D(5)
      REAL K
      COMMON NJ
      A(1)=-3.2656221735921635    $   A(2)=-1.019536199426184
      A(3)=-.196787330257926
      B(1)=.04158677121303    $   B(2)=.014404970304792
      B(3)=.004240024558143
      C(1)=-.000179660123307    $   C(2)=-.000072247077043
      C(3)=-.000029042912739
      D(1)=.000000340424969    $   D(2)=.000000158470271
      D(3)=.000000076307851
      DV=.1*F
      FLAGP=-1
      FLAGM=-1
      LOOP=0
      DO 1 J=1,NJ
    1 K(J)=A(J)+B(J)*TF+C(J)*TF*TF+D(J)*TF*TF*TF
  104 DO 8 J=1,NJ
      XF(J)=ZF(J)/(K(J)*FV/F+1.-FV/F)
    8 YF(J)=K(J)*XF(J)
      LOOP=LOOP+1
      IF (LOOP .GT. 100) STOP
      SUMX=0.
      DO 9 J=1,NJ
    9 SUMX=SUMX+XF(J)
      IF(ABS(SUMX-1.) .LT. .0000001) GO TO 30
      IF (SUMX-1.) 21,30,31
   21 IF(FLAGP .LT. 0) GO TO 22
      DV=DV/2.
   22 FV=FV+DV
      FLAGM=1
      GO TO 104
```

```
   31 IF(FLAGM .LT. 0) GO TO 32
      DV=DV/2.
   32 FV=FV-DV
      FLAGP=1
      GO TO 104
   30 CONTINUE
      RETURN
      END


      SUBROUTINE SPRINT(I,LOOP,NT,NF,XF,FV,YF,FL,TB,XB,YB,VB,X,T,Y,
     1V,L,TD,XD,YD,R,DIST,BOT,RR,QB,QD,TF,NN,LS,NS,XF1,YF1,NF1,FV1,
     2FL1,TF1)
C.....................................................................
C
C
C     SUBROUTINE SPRINT IS CALLED FROM MAIN TO PRINT THE
C     FINAL RESULTS.
C
C
C.....................................................................
      DIMENSION X(50,5),Y(50,5),XB(5),YB(5),XD(5),YD(5),L(50),V(50),
     1T(50),XF(5),YF(5),ZF(5),XS(5),XF1(5),YF1(5)
      REAL K,KB,KD,L,LS
      COMMON NJ
      PRINT 510,I,LOOP
      PRINT 511,NT,NF,TF,(XF(J),J=1,NJ),FL,(YF(J),J=1,NJ),FV
      IF(NN .EQ. 0) GO TO 1
      PRINT 518,NF1,TF1,(XF1(J),J=1,NJ),FL1,(YF1(J),J=1,NJ),FV1
    1 CONTINUE
      PRINT 512
      N=0
      PRINT 513,N,TB,(XB(J),J=1,NJ),(YB(J),J=1,NJ),VB
      DO 3 N=1,NT
    3 PRINT 514,N,T(N),(X(N,J),J=1,NJ),L(N),(Y(N,J),J=1,NJ),V(N)
      N=0
      PRINT 515,N,TD,(XD(J),J=1,NJ),R,(YD(J),J=1,NJ)
      IF(NN .EQ. 0) GO TO 2
      PRINT 517,NS,(X(NS,J),J=1,NJ),LS
    2 CONTINUE
      PRINT 516,DIST,BOT,RR,QB,QD
  510 FORMAT(/,1X,*RUN NO=*,I3,10X,*CONVERGED COLUMN ITERATIONS=*,I3//)
  511 FORMAT(/,1X,*NT=*,I3,10X,*NF=*,I3,10X,*TF=*,E10.4,//
     11X,*XF(1)=*,E15.5,10X,*XF(2)=*,E15.5,10X,*XF(3)=*,E15.5,10X,
     2*FL=*,E15.5,//1X,*YF(1)=*,E15.5,10X,*YF(2)=*,E15.5,10X,*YF(3)=*,
     3E15.5,10X,*FV=*,E15.5/)
  512 FORMAT(//,1X,* N        T                X(1)                X(2)
     1 X(3)          L                Y(1)                Y(2)
     2                Y(3)
     2       V   *)
  513 FORMAT(/,1X,I2,E13.5,3E15.5,13X,3E15.5,E13.5)
  514 FORMAT(/,1X,I2,E13.5,3E15.5,E13.5,3E15.5,E13.5)
  515 FORMAT(/,1X,I2,E13.5,3E15.5,E13.5,3E15.5)
  517 FORMAT(///,5X,*LIQUID SIDESTREAM DRAWOFF FROM TRAY NS=*,I3,//5X,
     1*SIDESTREAMS COMPOSITION AND FLOW RATE : *//1X,*X(NS,1)=*,E12.5,
     25X,*X(NS,2)=*,E12.5,5X,*X(NS,3)=*,E12.5,5X,*LS=*,E12.5///)
  516 FORMAT(//,1X,*DIST=*,E15.5,10X,*BOT=*,E15.5,10X,*RR=*,E14.5//,15X,
     1*QB=*,E15.5,1X,*BTU/HR*,10X,*QD=*,E15.5,1X,*BTU/HR*)
  518 FORMAT(/18X,*NF1=*,I3,10X,*TF1=*,E10.4,//1X,*XF1(1)=*,E15.5,10X,
     1*XF1(2)=*,E15.5,10X,*XF1(3)=*,E15.5,10X,*FL1=*,E15.5,//1X,*YF1(1)=
     2*,E15.5,10X,*YF1(2)=*,E15.5,10X,*YF1(3)=*,E15.5,10X,*FV1=*,E15.5/)
      RETURN
      END


      SUBROUTINE CLMSP(XF,TB,TD,V,QD,QB)
C.....................................................................
C
C     SUBROUTINE CLMSP IS CALLED FROM MAIN TO CALCULATE THE COLUMN*S
C     DIAMETER,THE CONDENSER*S AND REBOILER*S AREA,AND THE COST OF
C     STEAM AND COOLING WATER,GIVEN INFORMATION ABOUT THE MAXIMUM
C     VELOCITY OF THE VAPOR AT THE TOP OF THE TOWER,THE OVERALL HEAT
C     TRANSFER COEFFICIENTS OF THE CONDENSER AND THE REBOILER,THE
C     COST OF THE COOLING WATER AND THE STEAM USED,AND THE TOTAL
C     HOURS THAT THE UNIT WORKS PER YEAR
C
C.....................................................................
      DIMENSION MW(10),XF(10)
```

```
      COMMON NJ
      MOLECULAR WEIGHTS
      MW(1)=78.    $    MW(2)=92.    $    MW(3)=106.
      SPECIFY THE MAXIMUM VELOCITY OF VAPOR AT THE TOP OF THE TOWER
      (UVN) IN FT/SEC,AND  THE OVERALL HEAT TRANSFER COEFFICIENTS
      FOR THE CONDENSER(U1) AND THE REBOILER(U2),IN BTU/(HR*SQFT*DEG. F)
      UVN=2.5   $    U1=100.    $    U2=80.
      QB=ABS(QB)
      CALCULATE COLUMN*S DIAMETER
      MW1=0.
      DO 1 J=1,NJ
    1 MW1=MW1+XF(J)*MW(J)
      T=SQRT(TB*TD)
      RV=14.7*MW1/(10.731*(T+460.))
      VV=V*MW1
      QV=VV/(RV*3600.)
      A=QV/UVN
      DIAM=12.*SQRT(4.*A/3.141592654)
      CALCULATE CONDENSER*S AND REBOILER*S AREA
      AD=QD/(U1*(TD-90.))
      T1=417.35
      IF(TB .LE. 345.) T1=381.8
      AR=QB/(U2*(T1-TB))
      CALCULATE THE COST OF STEAM AND COOLING WATER
      THE COOLING WATER COSTS : $.06/10000LB
      THE STEAM HAS THE FOLLOWING SPECIFICATIONS :
      200 PSIA : T1=381.8 DEG F,HL1=842.8 BTU/LB-MOLE,COST=$2.0/1000LB
      300 PSIA : T2=417.3 DEG F,HL2=808.9 BTU/LB-MOLE,COST=$2.2/1000LB
      THE UNIT WORKS 8500 HRS/YEAR
      CS=QB*(2.2/1000.)*8500./808.9
      IF(T1 .EQ. 381.8) CS=QB*(2.0/1000.)*8500./842.8
      CCW=QD*(.06/10000.)*8500./50.
      PRINT 700,DIAM,AR,AD,CCW,CS
  700 FORMAT(///,20X,*COLUMNS DIAMETER=*,F8.4,1X,*INCHES*,//,10X,
     1*REBOILERS AREA=*,F8.2,1X,*SQFT*,10X,*CONDENSERS AREA=*,F8.2,1X,
     2*SQFT*,//,10X,*COST OF COOLING WATER=*,F8.0,1X,*DOLLARS*,5X,*COST
     3OF STEAM=*,F8.0,1X,*DOLLARS*///)
      RETURN
      END
```

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